



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 04:40 AM UTC

PDB ID : 3I5I / pdb_00003i5i
Title : The crystal structure of squid myosin S1 in the presence of SO4 2-
Authors : Yang, Y.; Gourinath, S.; Kovacs, M.; Nyitray, L.; Reutzel, R.; Himmel, D.M.; O'Neill-Hennessey, E.; Reshetnikova, L.; Szent-Gyorgyi, A.G.; Brown, J.H.; Cohen, C.
Deposited on : 2009-07-05
Resolution : 3.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

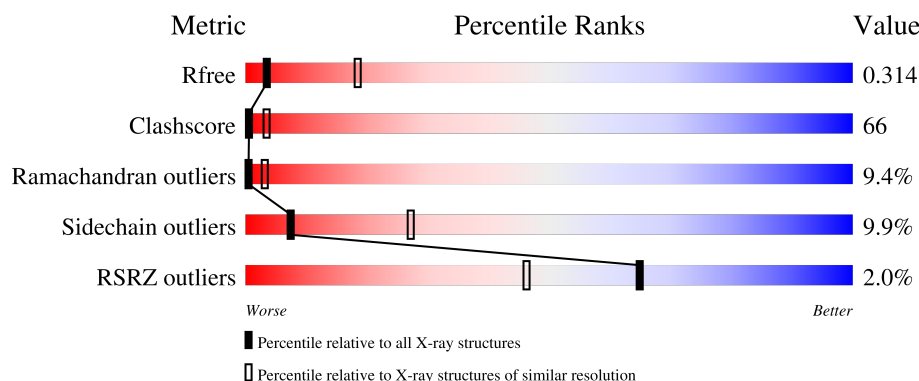
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

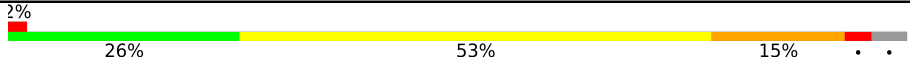
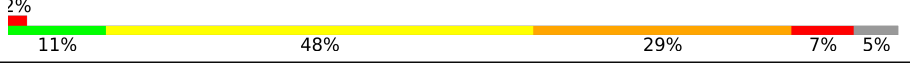
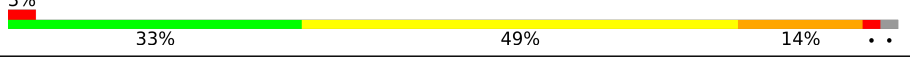
The reported resolution of this entry is 3.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	839	
2	B	153	
3	C	159	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SO4	A	1001	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8904 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Myosin heavy chain isoform A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	808	Total	C	N	O	S	0	0	0
			6493	4150	1111	1193	39			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	238	LYS	GLU	conflict	UNP O44934
A	744	ALA	VAL	conflict	UNP O44934

- Molecule 2 is a protein called Myosin regulatory light chain LC-2, mantle muscle.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	145	Total	C	N	O	S	0	0	0
			1166	733	191	233	9			

- Molecule 3 is a protein called Myosin catalytic light chain LC-1, mantle muscle.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	156	Total	C	N	O	S	0	0	0
			1239	773	203	253	10			

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		

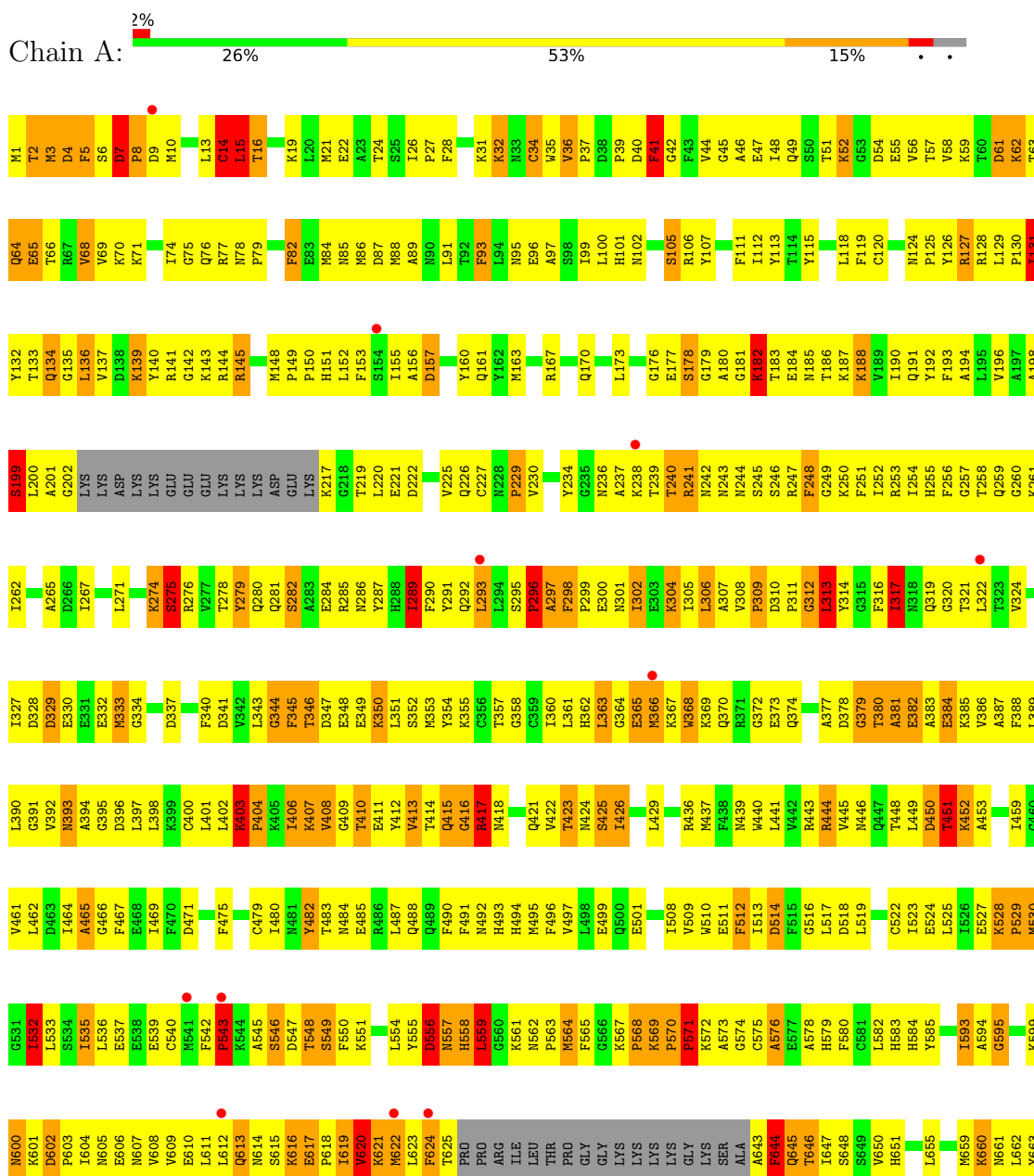
- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

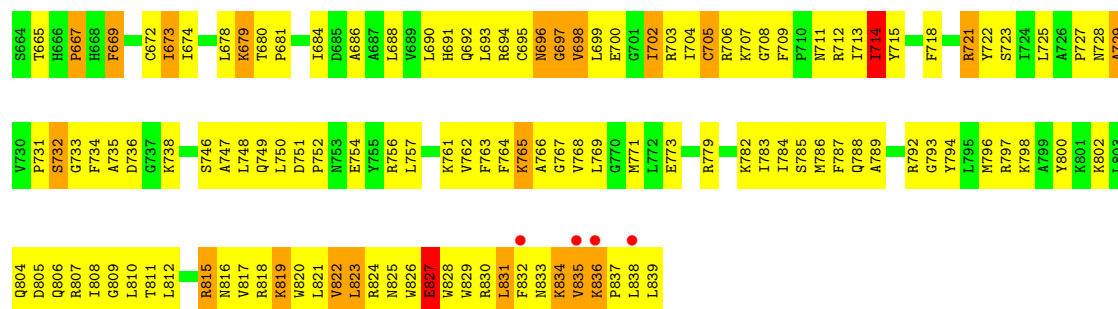
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	1	Total	Ca	0	0
			1	1		

3 Residue-property plots

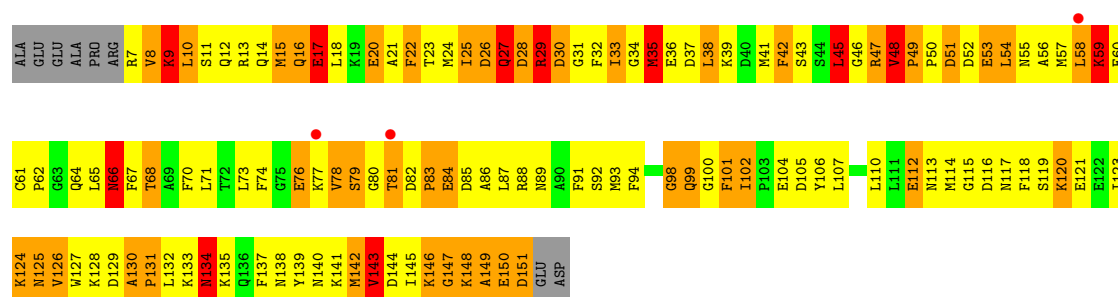
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

● Molecule 1: Myosin heavy chain isoform A

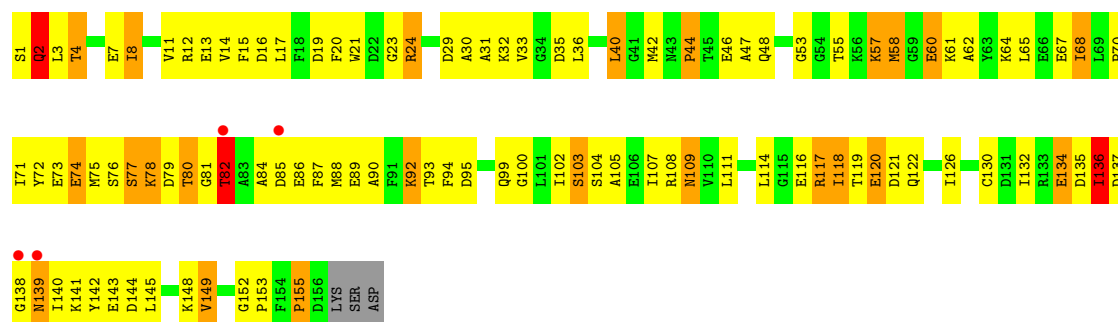




- Molecule 2: Myosin regulatory light chain LC-2, mantle muscle



- Molecule 3: Myosin catalytic light chain LC-1, mantle muscle



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	195.19Å 100.15Å 80.19Å 90.00° 105.45° 90.00°	Depositor
Resolution (Å)	50.00 – 3.30 50.00 – 3.30	Depositor EDS
% Data completeness (in resolution range)	97.2 (50.00-3.30) 97.2 (50.00-3.30)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.33 (at 3.33Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.262 , 0.330 0.251 , 0.314	Depositor DCC
R_{free} test set	2180 reflections (9.94%)	wwPDB-VP
Wilson B-factor (Å ²)	69.7	Xtriage
Anisotropy	0.533	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 75.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	8904	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, CA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.66	1/6631 (0.0%)	1.30	115/8938 (1.3%)
2	B	0.70	1/1186 (0.1%)	1.70	29/1588 (1.8%)
3	C	0.73	0/1258	1.46	22/1687 (1.3%)
All	All	0.68	2/9075 (0.0%)	1.38	166/12213 (1.4%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	766	ALA	CA-CB	-5.54	1.45	1.53
2	B	28	ASP	CA-C	-5.20	1.46	1.52

All (166) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	28	ASP	N-CA-C	21.82	144.32	109.85
2	B	100	GLY	N-CA-C	-20.06	89.09	114.37
3	C	2	GLN	N-CA-C	13.95	140.51	110.80
2	B	27	GLN	N-CA-C	-13.62	81.79	110.80
2	B	10	LEU	N-CA-C	-11.53	88.50	108.56
3	C	58	MET	N-CA-C	11.31	127.42	113.50
2	B	149	ALA	N-CA-C	-11.29	95.79	112.04
1	A	620	VAL	N-CA-C	-11.21	102.82	111.90
3	C	138	GLY	N-CA-C	-11.11	86.84	113.18
1	A	645	GLN	N-CA-C	11.08	126.14	109.63
2	B	76	GLU	N-CA-C	-10.41	101.63	114.75
3	C	74	GLU	N-CA-C	-10.03	99.90	111.03
3	C	80	THR	N-CA-C	-9.57	95.53	109.11
3	C	81	GLY	N-CA-C	-9.31	103.11	114.66
1	A	304	LYS	N-CA-C	-9.29	101.11	111.14
2	B	83	PRO	N-CA-C	9.06	123.90	111.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	557	ASN	N-CA-C	8.95	121.85	111.11
1	A	451	THR	N-CA-C	-8.90	95.24	109.39
1	A	297	ALA	N-CA-C	-8.59	92.50	110.80
1	A	561	LYS	N-CA-C	8.44	123.13	113.01
1	A	182	LYS	N-CA-C	-8.31	101.12	111.75
1	A	439	ASN	N-CA-C	-8.25	102.23	111.14
1	A	673	ILE	N-CA-C	8.23	119.55	108.27
2	B	151	ASP	CA-C-O	7.97	134.35	120.80
1	A	333	MET	N-CA-C	-7.89	102.75	112.38
3	C	71	ILE	N-CA-C	-7.84	103.16	110.53
1	A	471	ASP	N-CA-C	-7.82	103.19	112.89
1	A	365	GLU	N-CA-C	-7.77	101.92	111.40
1	A	697	GLY	N-CA-C	-7.75	103.79	114.64
1	A	4	ASP	N-CA-C	-7.71	95.84	108.41
1	A	345	PHE	N-CA-C	7.70	121.78	108.76
2	B	101	PHE	N-CA-C	7.66	127.11	110.80
2	B	68	THR	N-CA-C	-7.49	103.12	111.28
2	B	47	ARG	N-CA-C	7.44	126.64	110.80
1	A	595	GLY	N-CA-C	7.43	125.21	115.40
1	A	14	CYS	N-CA-C	7.34	126.44	110.80
1	A	381	ALA	N-CA-C	-7.27	103.04	110.97
1	A	34	CYS	N-CA-C	7.24	118.09	107.88
1	A	199	SER	N-CA-C	7.16	126.06	110.80
1	A	7	ASP	CA-C-N	7.15	128.78	119.84
1	A	7	ASP	C-N-CA	7.15	128.78	119.84
1	A	393	ASN	N-CA-C	7.07	120.90	107.75
1	A	255	HIS	N-CA-C	7.03	119.60	110.53
2	B	126	VAL	N-CA-C	6.99	117.83	111.81
1	A	646	THR	N-CA-C	6.98	119.78	109.24
1	A	834	LYS	N-CA-C	-6.95	102.81	112.12
2	B	120	LYS	N-CA-C	-6.94	103.92	112.38
2	B	17	GLU	N-CA-C	-6.90	103.78	111.71
2	B	35	MET	N-CA-C	-6.89	103.00	111.33
2	B	78	VAL	N-CA-C	6.86	119.63	111.05
1	A	558	HIS	N-CA-C	6.85	121.32	112.41
1	A	831	LEU	N-CA-C	6.83	118.42	110.97
1	A	313	LEU	N-CA-C	6.82	125.33	110.80
1	A	535	ILE	N-CA-C	-6.78	103.87	110.72
1	A	403	LYS	CA-C-N	6.76	128.29	119.84
1	A	403	LYS	C-N-CA	6.76	128.29	119.84
1	A	617	GLU	CA-C-N	-6.74	111.96	118.97
1	A	617	GLU	C-N-CA	-6.74	111.96	118.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	131	ILE	N-CA-C	6.71	123.29	109.34
1	A	807	ARG	N-CA-C	-6.63	103.54	111.69
2	B	45	LEU	N-CA-C	-6.56	103.33	112.45
1	A	241	ARG	N-CA-C	6.54	120.17	112.72
1	A	279	TYR	N-CA-C	6.47	118.93	108.32
1	A	482	TYR	N-CA-C	-6.45	104.25	111.28
1	A	15	LEU	N-CA-C	-6.40	97.17	110.80
1	A	401	LEU	N-CA-C	-6.40	104.17	112.68
1	A	219	THR	N-CA-C	-6.36	101.10	110.52
1	A	385	LYS	N-CA-C	-6.34	104.29	111.14
3	C	82	THR	N-CA-C	6.34	124.30	110.80
1	A	139	LYS	N-CA-C	-6.21	104.97	112.54
2	B	16	GLN	N-CA-C	-6.21	105.84	113.41
1	A	562	ASN	CA-C-N	6.20	125.68	119.24
1	A	562	ASN	C-N-CA	6.20	125.68	119.24
1	A	721	ARG	N-CA-C	6.15	120.91	113.41
1	A	403	LYS	N-CA-C	6.11	123.32	109.81
2	B	100	GLY	CA-C-O	6.09	125.42	119.27
1	A	145	ARG	N-CA-C	6.06	123.70	110.80
1	A	469	ILE	N-CA-C	-6.02	98.81	107.78
1	A	512	PHE	N-CA-C	6.00	119.01	108.75
1	A	444	ARG	N-CA-C	5.98	117.67	111.03
2	B	131	PRO	N-CA-C	-5.98	100.80	110.55
1	A	729	ALA	N-CA-C	5.97	120.04	112.87
1	A	62	LYS	N-CA-C	5.97	123.52	110.80
1	A	613	GLN	N-CA-C	-5.96	104.15	112.25
1	A	410	THR	N-CA-C	-5.95	100.56	109.96
3	C	136	ILE	CA-C-N	-5.94	113.62	123.37
3	C	136	ILE	C-N-CA	-5.94	113.62	123.37
1	A	602	ASP	CA-C-N	5.90	125.66	119.76
1	A	602	ASP	C-N-CA	5.90	125.66	119.76
1	A	198	ALA	N-CA-C	-5.90	106.12	113.38
1	A	733	GLY	N-CA-C	5.88	120.30	112.77
1	A	559	LEU	N-CA-C	5.86	123.27	110.80
1	A	452	LYS	N-CA-C	5.82	118.96	110.17
1	A	569	LYS	CA-C-N	5.82	126.37	120.38
1	A	569	LYS	C-N-CA	5.82	126.37	120.38
1	A	3	MET	CB-CG-SD	-5.82	95.25	112.70
1	A	600	ASN	N-CA-C	5.81	119.55	112.23
2	B	49	PRO	N-CA-C	5.81	117.79	110.70
2	B	143	VAL	N-CA-C	-5.81	104.00	110.62
1	A	281	GLN	N-CA-C	5.78	117.86	109.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	57	LYS	N-CA-C	5.78	118.44	109.60
3	C	53	GLY	N-CA-C	5.78	119.76	113.58
1	A	378	ASP	N-CA-C	-5.76	103.61	110.41
3	C	40	LEU	N-CA-C	-5.75	105.75	112.89
1	A	669	PHE	N-CA-C	5.69	117.69	108.41
1	A	93	PHE	N-CA-C	-5.66	99.19	108.41
2	B	8	VAL	CB-CA-C	-5.62	102.07	111.29
1	A	836	LYS	CA-C-N	-5.62	112.81	119.84
1	A	836	LYS	C-N-CA	-5.62	112.81	119.84
1	A	798	LYS	N-CA-C	-5.60	104.67	112.45
1	A	28	PHE	N-CA-C	5.58	117.01	108.52
1	A	222	ASP	N-CA-C	5.57	118.54	111.69
1	A	21	MET	N-CA-C	-5.56	104.60	111.33
1	A	157	ASP	N-CA-C	-5.53	105.26	111.28
1	A	344	GLY	CA-C-N	-5.51	114.26	122.74
1	A	344	GLY	C-N-CA	-5.51	114.26	122.74
1	A	528	LYS	N-CA-C	5.50	121.96	109.81
3	C	1	SER	CA-C-N	5.49	132.03	121.54
3	C	1	SER	C-N-CA	5.49	132.03	121.54
1	A	347	ASP	N-CA-C	-5.48	106.29	112.87
1	A	379	GLY	N-CA-C	-5.47	103.20	110.58
3	C	120	GLU	N-CA-C	-5.43	105.26	111.07
3	C	134	GLU	N-CA-C	-5.40	101.77	110.14
1	A	177	GLU	N-CA-C	5.39	116.97	109.31
1	A	757	LEU	N-CA-C	5.38	117.51	108.73
1	A	453	ALA	N-CA-C	-5.38	99.91	108.30
3	C	64	LYS	N-CA-C	-5.37	102.93	110.35
1	A	289	ILE	N-CA-C	5.37	116.74	110.62
1	A	368	TRP	N-CA-C	5.37	117.25	108.76
1	A	501	GLU	N-CA-C	-5.36	105.36	111.14
3	C	105	ALA	N-CA-C	-5.36	104.89	111.75
1	A	248	PHE	CA-C-N	-5.33	117.77	122.73
1	A	248	PHE	C-N-CA	-5.33	117.77	122.73
1	A	409	GLY	N-CA-C	-5.32	100.56	113.18
1	A	113	TYR	N-CA-C	5.32	118.16	109.59
1	A	89	ALA	N-CA-C	-5.32	105.56	111.36
1	A	296	PRO	N-CA-C	5.31	123.41	112.47
1	A	705	CYS	N-CA-C	-5.30	105.50	111.28
1	A	41	PHE	N-CA-C	5.28	119.47	108.53
3	C	116	GLU	N-CA-C	-5.26	100.22	108.63
3	C	109	ASN	N-CA-C	-5.25	105.45	111.07
1	A	384	GLU	N-CA-C	-5.24	106.39	112.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	571	PRO	N-CA-C	5.23	123.24	112.47
1	A	735	ALA	N-CA-C	5.22	118.21	110.48
1	A	614	ASN	N-CA-C	5.22	117.19	108.99
2	B	112	GLU	N-CA-C	5.21	117.04	111.36
3	C	114	LEU	N-CA-C	5.19	117.78	110.14
1	A	509	VAL	N-CA-C	5.18	115.68	108.84
1	A	16	THR	N-CA-C	5.18	118.14	110.48
1	A	528	LYS	CA-C-N	5.17	126.31	119.84
1	A	528	LYS	C-N-CA	5.17	126.31	119.84
2	B	28	ASP	CB-CA-C	-5.14	99.68	109.66
1	A	134	GLN	N-CA-C	-5.12	106.98	113.18
1	A	136	LEU	N-CA-C	-5.11	105.62	111.14
1	A	403	LYS	C-N-CD	-5.10	104.08	125.00
1	A	660	LYS	N-CA-C	-5.10	105.16	111.33
2	B	100	GLY	CA-C-N	5.07	131.22	121.54
2	B	100	GLY	C-N-CA	5.07	131.22	121.54
1	A	617	GLU	N-CA-C	5.06	120.45	113.77
1	A	714	ILE	N-CA-C	-5.06	103.05	109.58
1	A	286	ASN	N-CA-C	-5.06	103.92	110.19
1	A	82	PHE	N-CA-C	5.02	119.38	113.16
2	B	102	ILE	N-CA-C	5.02	119.72	108.88
2	B	29	ARG	N-CA-C	-5.01	100.13	110.80
1	A	32	LYS	N-CA-C	5.01	121.46	110.80
1	A	819	LYS	N-CA-C	-5.00	105.91	111.36

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6493	0	6496	841	0
2	B	1166	0	1125	256	1
3	C	1239	0	1190	142	0
4	A	5	0	0	4	0
5	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	8904	0	8811	1173	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 66.

All (1173) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:ARG:NH2	1:A:199:SER:HB3	1.54	1.20
1:A:191:GLN:HG2	1:A:221:GLU:HG2	1.19	1.18
2:B:26:ASP:OD1	2:B:28:ASP:HB2	1.47	1.15
1:A:259:GLN:H	1:A:261:LYS:HE2	1.13	1.12
1:A:365:GLU:O	1:A:367:LYS:HD3	1.50	1.11
1:A:786:MET:HE1	3:C:80:THR:O	1.49	1.09
1:A:413:VAL:HG13	1:A:415:GLN:HB2	1.33	1.08
1:A:190:ILE:HG12	1:A:254:ILE:HD11	1.36	1.05
2:B:7:ARG:O	2:B:78:VAL:HG11	1.54	1.05
1:A:572:LYS:HB3	1:A:575:CYS:HB2	1.36	1.04
2:B:142:MET:HE1	2:B:146:LYS:HD3	1.38	1.04
2:B:84:GLU:HG3	2:B:85:ASP:H	1.22	1.03
1:A:84:MET:HE1	1:A:105:SER:HB2	1.37	1.02
1:A:802:LYS:HE2	1:A:806:GLN:NE2	1.75	1.01
1:A:316:PHE:HE1	1:A:364:GLY:HA2	1.21	1.00
1:A:572:LYS:H	1:A:575:CYS:HB3	1.25	1.00
1:A:404:PRO:HB3	1:A:607:ASN:HD22	1.27	1.00
1:A:620:VAL:O	1:A:624:PHE:HB2	1.62	1.00
2:B:23:THR:O	2:B:26:ASP:HB2	1.62	0.99
1:A:78:ASN:OD1	1:A:93:PHE:HB2	1.63	0.99
1:A:550:PHE:HE2	1:A:593:ILE:HD12	1.29	0.97
1:A:404:PRO:HB3	1:A:607:ASN:ND2	1.79	0.96
2:B:120:LYS:HA	2:B:123:ILE:HD12	1.45	0.96
1:A:141:ARG:HH22	1:A:199:SER:HB3	1.21	0.96
1:A:2:THR:HG21	1:A:143:LYS:NZ	1.80	0.95
2:B:25:ILE:O	2:B:37:ASP:HB3	1.67	0.95
1:A:88:MET:HE3	1:A:102:ASN:HB3	1.49	0.95
1:A:571:PRO:HB2	1:A:575:CYS:HB3	1.46	0.94
1:A:316:PHE:CE1	1:A:364:GLY:HA2	2.02	0.94
1:A:750:LEU:HD13	1:A:771:MET:HE1	1.50	0.94
1:A:817:VAL:HA	2:B:146:LYS:HZ1	1.33	0.93
1:A:316:PHE:CE1	1:A:364:GLY:CA	2.52	0.93
1:A:317:ILE:HD12	1:A:361:LEU:HD21	1.51	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:MET:HE3	1:A:386:VAL:HG21	1.52	0.92
1:A:316:PHE:HE1	1:A:364:GLY:CA	1.82	0.92
1:A:403:LYS:N	1:A:404:PRO:HD2	1.80	0.91
1:A:167:ARG:HH22	1:A:258:THR:HG23	1.35	0.91
2:B:26:ASP:OD1	2:B:28:ASP:CB	2.17	0.91
2:B:35:MET:HE3	2:B:54:LEU:HD23	1.52	0.91
3:C:4:THR:HG23	3:C:7:GLU:HG3	1.51	0.91
1:A:2:THR:HG21	1:A:143:LYS:HZ1	1.31	0.90
3:C:3:LEU:HD21	3:C:73:GLU:HB3	1.53	0.89
1:A:190:ILE:CG1	1:A:254:ILE:HD11	2.02	0.89
1:A:293:LEU:HA	1:A:333:MET:HE3	1.55	0.89
3:C:130:CYS:O	3:C:148:LYS:HD3	1.73	0.88
1:A:436:ARG:HH11	1:A:623:LEU:HA	1.37	0.88
1:A:569:LYS:HD2	1:A:569:LYS:O	1.73	0.88
1:A:3:MET:HE1	1:A:14:CYS:SG	2.14	0.88
2:B:8:VAL:C	2:B:10:LEU:H	1.79	0.88
1:A:278:THR:HG22	1:A:316:PHE:CD2	2.08	0.88
3:C:153:PRO:O	3:C:155:PRO:HD3	1.74	0.87
1:A:13:LEU:HD11	1:A:151:HIS:HD2	1.39	0.87
2:B:24:MET:C	2:B:26:ASP:H	1.79	0.87
1:A:196:VAL:O	1:A:199:SER:HB2	1.74	0.86
1:A:406:ILE:HD12	1:A:414:THR:HG21	1.57	0.86
1:A:796:MET:HE3	3:C:35:ASP:CG	2.00	0.86
1:A:191:GLN:HG2	1:A:221:GLU:CG	2.04	0.86
1:A:413:VAL:HG13	1:A:415:GLN:CB	2.05	0.86
1:A:608:VAL:O	1:A:612:LEU:HG	1.75	0.86
1:A:259:GLN:N	1:A:261:LYS:HE2	1.90	0.85
1:A:297:ALA:HB3	1:A:298:PHE:CE1	2.11	0.85
1:A:836:LYS:NZ	2:B:21:ALA:HB2	1.90	0.85
2:B:9:LYS:HA	2:B:9:LYS:HE3	1.58	0.85
1:A:572:LYS:O	1:A:572:LYS:HG3	1.74	0.85
3:C:90:ALA:O	3:C:93:THR:HG22	1.77	0.84
3:C:103:SER:HA	3:C:139:ASN:CG	2.02	0.84
1:A:836:LYS:HZ2	2:B:21:ALA:HB2	1.38	0.83
1:A:298:PHE:HB3	1:A:301:ASN:HD22	1.43	0.83
1:A:230:VAL:HG11	1:A:441:LEU:HD11	1.59	0.83
1:A:406:ILE:HG22	1:A:407:LYS:N	1.91	0.83
3:C:88:MET:HE3	3:C:142:TYR:HE1	1.43	0.83
1:A:406:ILE:HG22	1:A:407:LYS:H	1.42	0.82
1:A:317:ILE:HD12	1:A:361:LEU:CD2	2.09	0.82
1:A:278:THR:HG22	1:A:316:PHE:CE2	2.13	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:400:CYS:HA	1:A:404:PRO:HD3	1.59	0.82
1:A:194:ALA:HA	1:A:262:ILE:CD1	2.09	0.82
1:A:391:GLY:O	1:A:615:SER:HB3	1.79	0.82
1:A:550:PHE:CE2	1:A:593:ILE:HD12	2.15	0.82
1:A:259:GLN:HB2	1:A:261:LYS:HD3	1.59	0.82
1:A:600:ASN:HD21	1:A:648:SER:H	1.29	0.81
2:B:8:VAL:O	2:B:10:LEU:N	2.13	0.81
1:A:47:GLU:O	1:A:58:VAL:HG13	1.79	0.81
1:A:555:TYR:HE2	1:A:567:LYS:HD2	1.45	0.80
1:A:610:GLU:O	1:A:613:GLN:HB2	1.79	0.80
3:C:132:ILE:CD1	3:C:145:LEU:HA	2.11	0.80
2:B:131:PRO:HB3	2:B:141:LYS:CD	2.11	0.80
2:B:11:SER:O	2:B:15:MET:HG3	1.82	0.80
1:A:826:TRP:O	1:A:829:TRP:N	2.14	0.79
1:A:362:HIS:C	1:A:364:GLY:H	1.89	0.79
1:A:4:ASP:C	1:A:6:SER:H	1.89	0.79
1:A:817:VAL:HA	2:B:146:LYS:NZ	1.97	0.79
1:A:316:PHE:CD1	1:A:364:GLY:HA3	2.18	0.78
1:A:292:GLN:HB3	1:A:333:MET:HE2	1.64	0.78
1:A:120:CYS:HB2	1:A:155:ILE:HD11	1.64	0.78
1:A:404:PRO:HB2	1:A:414:THR:OG1	1.83	0.78
2:B:29:ARG:HG3	2:B:32:PHE:HB2	1.66	0.78
2:B:53:GLU:O	2:B:56:ALA:N	2.16	0.78
1:A:417:ARG:NE	1:A:417:ARG:H	1.81	0.78
1:A:828:TRP:CZ2	2:B:57:MET:HB3	2.18	0.77
1:A:403:LYS:H	1:A:404:PRO:HD2	1.46	0.77
1:A:119:PHE:CE1	1:A:698:VAL:HA	2.18	0.77
1:A:280:GLN:HB2	1:A:319:GLN:HB2	1.66	0.77
1:A:599:LYS:O	1:A:647:ILE:HD12	1.85	0.77
2:B:24:MET:C	2:B:26:ASP:N	2.35	0.77
1:A:343:LEU:CD1	1:A:445:VAL:HG12	2.14	0.77
2:B:29:ARG:HH21	2:B:34:GLY:HA2	1.49	0.77
1:A:368:TRP:CZ3	1:A:402:LEU:HD21	2.20	0.77
1:A:374:GLN:CD	1:A:415:GLN:HE21	1.92	0.76
1:A:834:LYS:HD2	2:B:45:LEU:HD13	1.67	0.76
1:A:298:PHE:CE1	1:A:333:MET:HG3	2.20	0.76
1:A:834:LYS:HD2	2:B:45:LEU:CD1	2.15	0.76
2:B:101:PHE:HD2	2:B:139:TYR:CD2	2.04	0.76
3:C:103:SER:HA	3:C:139:ASN:CB	2.16	0.76
3:C:135:ASP:O	3:C:136:ILE:C	2.29	0.76
2:B:24:MET:O	2:B:26:ASP:N	2.19	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:390:LEU:HD22	1:A:619:ILE:HD11	1.68	0.75
3:C:117:ARG:HG3	3:C:117:ARG:HH11	1.50	0.75
1:A:173:LEU:HD22	1:A:462:LEU:HD23	1.69	0.75
1:A:551:LYS:HG2	1:A:555:TYR:CE1	2.21	0.75
1:A:725:LEU:HD13	1:A:748:LEU:HD11	1.67	0.75
1:A:293:LEU:HD23	1:A:333:MET:HE1	1.69	0.75
1:A:88:MET:CE	1:A:99:ILE:HA	2.17	0.75
3:C:78:LYS:HA	3:C:78:LYS:HE3	1.69	0.75
1:A:221:GLU:O	1:A:225:VAL:HG23	1.86	0.75
1:A:731:PRO:HG2	1:A:734:PHE:HD1	1.52	0.75
2:B:34:GLY:H	2:B:37:ASP:HB2	1.52	0.75
1:A:343:LEU:HD13	1:A:445:VAL:HG12	1.66	0.74
1:A:10:MET:HB3	1:A:14:CYS:HB2	1.70	0.74
1:A:731:PRO:HG2	1:A:734:PHE:CD1	2.22	0.74
2:B:13:ARG:HD2	2:B:13:ARG:N	2.00	0.74
2:B:142:MET:CE	2:B:146:LYS:HD3	2.15	0.74
3:C:4:THR:HG23	3:C:7:GLU:CG	2.16	0.74
3:C:136:ILE:HG22	3:C:137:ASP:H	1.51	0.74
2:B:150:GLU:HG2	2:B:151:ASP:N	2.02	0.74
1:A:296:PRO:HD2	1:A:330:GLU:HG2	1.70	0.74
1:A:406:ILE:CD1	1:A:414:THR:HG21	2.15	0.74
1:A:819:LYS:HE3	2:B:76:GLU:O	1.88	0.74
1:A:831:LEU:HD21	2:B:42:PHE:CE1	2.22	0.74
1:A:194:ALA:HA	1:A:262:ILE:HD12	1.69	0.74
1:A:236:ASN:HB3	1:A:244:ASN:ND2	2.03	0.73
1:A:572:LYS:N	1:A:575:CYS:HB3	2.01	0.73
1:A:133:THR:HG22	1:A:135:GLY:H	1.52	0.73
1:A:414:THR:O	1:A:416:GLY:N	2.21	0.73
1:A:406:ILE:CG1	1:A:414:THR:HG21	2.19	0.73
1:A:568:PRO:HG3	1:A:578:ALA:HB3	1.70	0.73
1:A:345:PHE:CD2	1:A:444:ARG:NH2	2.56	0.73
2:B:23:THR:C	2:B:26:ASP:HB2	2.14	0.73
1:A:49:GLN:HB2	1:A:57:THR:HG22	1.68	0.73
1:A:391:GLY:O	1:A:615:SER:CB	2.37	0.72
1:A:417:ARG:HE	1:A:417:ARG:N	1.87	0.72
2:B:29:ARG:NH2	2:B:34:GLY:CA	2.52	0.72
1:A:64:GLN:OE1	1:A:64:GLN:HA	1.88	0.72
1:A:141:ARG:CZ	1:A:199:SER:HB3	2.19	0.72
1:A:754:GLU:HA	1:A:754:GLU:OE1	1.89	0.72
2:B:29:ARG:CZ	2:B:34:GLY:HA3	2.18	0.72
1:A:234:TYR:CZ	1:A:289:ILE:HD12	2.23	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:563:PRO:HG2	1:A:564:MET:HE2	1.71	0.72
2:B:149:ALA:O	2:B:150:GLU:HB2	1.90	0.72
1:A:694:ARG:HG2	1:A:699:LEU:HD12	1.70	0.72
1:A:786:MET:SD	3:C:82:THR:OG1	2.47	0.72
1:A:365:GLU:OE1	1:A:365:GLU:HA	1.89	0.72
1:A:366:MET:CE	1:A:386:VAL:HG21	2.18	0.72
1:A:436:ARG:NH1	1:A:623:LEU:HA	2.03	0.72
1:A:2:THR:HG22	1:A:2:THR:O	1.88	0.72
1:A:571:PRO:HB2	1:A:575:CYS:CB	2.19	0.71
2:B:35:MET:HE3	2:B:54:LEU:CD2	2.19	0.71
1:A:36:VAL:CG2	1:A:69:VAL:HG21	2.19	0.71
2:B:99:GLN:C	2:B:101:PHE:H	1.81	0.71
1:A:369:LYS:HD2	1:A:370:GLN:H	1.55	0.71
2:B:67:PHE:HA	2:B:70:PHE:HB2	1.73	0.71
1:A:346:THR:HG22	1:A:348:GLU:H	1.56	0.71
1:A:136:LEU:HD23	1:A:139:LYS:HD2	1.73	0.71
2:B:14:GLN:HE22	2:B:81:THR:HG23	1.55	0.71
1:A:293:LEU:HD23	1:A:333:MET:CE	2.20	0.71
1:A:313:LEU:H	1:A:313:LEU:HD23	1.56	0.71
1:A:362:HIS:O	1:A:364:GLY:N	2.24	0.71
2:B:101:PHE:HB2	2:B:137:PHE:O	1.90	0.71
1:A:407:LYS:O	1:A:408:VAL:HG23	1.91	0.70
1:A:415:GLN:O	1:A:417:ARG:N	2.24	0.70
2:B:46:GLY:O	2:B:47:ARG:HG2	1.90	0.70
2:B:11:SER:O	2:B:15:MET:CG	2.39	0.70
2:B:26:ASP:OD1	2:B:28:ASP:CG	2.34	0.70
1:A:708:GLY:O	1:A:765:LYS:HE2	1.92	0.70
1:A:831:LEU:HD21	2:B:42:PHE:CZ	2.27	0.70
2:B:131:PRO:HB3	2:B:141:LYS:CE	2.22	0.70
3:C:4:THR:CG2	3:C:7:GLU:HG3	2.21	0.69
3:C:136:ILE:HG22	3:C:137:ASP:N	2.07	0.69
1:A:464:ILE:HG23	1:A:465:ALA:N	2.07	0.69
1:A:782:LYS:O	1:A:786:MET:HG3	1.92	0.69
2:B:9:LYS:HA	2:B:9:LYS:CE	2.14	0.69
2:B:10:LEU:HB2	2:B:78:VAL:HG21	1.75	0.69
2:B:23:THR:O	2:B:26:ASP:CB	2.38	0.69
1:A:362:HIS:C	1:A:364:GLY:N	2.49	0.69
1:A:510:TRP:CE2	1:A:512:PHE:HB2	2.28	0.69
2:B:7:ARG:C	2:B:9:LYS:N	2.42	0.69
1:A:312:GLY:O	1:A:314:TYR:N	2.25	0.69
2:B:8:VAL:C	2:B:10:LEU:N	2.50	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:15:MET:SD	2:B:71:LEU:HD13	2.32	0.69
2:B:67:PHE:CZ	2:B:71:LEU:HD11	2.28	0.69
3:C:132:ILE:HD11	3:C:145:LEU:HA	1.73	0.69
1:A:525:LEU:O	1:A:532:ILE:HG13	1.93	0.69
1:A:620:VAL:HG12	1:A:624:PHE:CE1	2.28	0.69
1:A:293:LEU:CA	1:A:333:MET:HE3	2.22	0.68
1:A:415:GLN:O	1:A:416:GLY:C	2.34	0.68
2:B:88:ARG:HE	2:B:143:VAL:HG11	1.57	0.68
1:A:316:PHE:O	1:A:317:ILE:HG13	1.92	0.68
3:C:11:VAL:HA	3:C:40:LEU:HD21	1.75	0.68
1:A:345:PHE:HB3	1:A:349:GLU:OE1	1.92	0.68
1:A:537:GLU:O	1:A:540:CYS:HB2	1.93	0.68
1:A:417:ARG:H	1:A:417:ARG:HE	1.38	0.68
1:A:822:VAL:HG12	1:A:823:LEU:N	2.08	0.68
1:A:609:VAL:O	1:A:613:GLN:HG3	1.94	0.68
1:A:806:GLN:HG2	2:B:93:MET:HE2	1.75	0.68
1:A:251:PHE:HA	1:A:461:VAL:O	1.93	0.67
1:A:194:ALA:HA	1:A:262:ILE:HD11	1.75	0.67
1:A:575:CYS:O	1:A:576:ALA:O	2.13	0.67
1:A:5:PHE:O	1:A:16:THR:HG22	1.94	0.67
1:A:617:GLU:O	1:A:620:VAL:HG23	1.95	0.67
2:B:12:GLN:HB3	2:B:13:ARG:HH11	1.58	0.67
1:A:298:PHE:HB3	1:A:301:ASN:ND2	2.09	0.67
1:A:513:ILE:HG12	1:A:517:LEU:HD12	1.75	0.67
3:C:100:GLY:HA2	3:C:142:TYR:CZ	2.29	0.67
1:A:466:GLY:O	1:A:484:ASN:ND2	2.28	0.67
1:A:51:THR:HG22	1:A:52:LYS:N	2.10	0.67
1:A:88:MET:HE1	1:A:99:ILE:HA	1.75	0.67
3:C:103:SER:HA	3:C:139:ASN:HB3	1.76	0.67
2:B:124:LYS:O	2:B:126:VAL:N	2.27	0.67
2:B:149:ALA:O	2:B:150:GLU:CB	2.43	0.67
3:C:44:PRO:HA	3:C:48:GLN:OE1	1.92	0.67
3:C:100:GLY:HA2	3:C:142:TYR:CE2	2.30	0.67
2:B:124:LYS:C	2:B:126:VAL:N	2.52	0.66
1:A:619:ILE:HG22	1:A:619:ILE:O	1.95	0.66
1:A:568:PRO:HG3	1:A:578:ALA:CB	2.26	0.66
1:A:729:ALA:HA	3:C:85:ASP:OD1	1.95	0.66
1:A:155:ILE:HG22	1:A:155:ILE:O	1.95	0.66
1:A:365:GLU:O	1:A:367:LYS:CD	2.38	0.66
2:B:81:THR:HG23	2:B:81:THR:O	1.96	0.66
1:A:239:THR:O	1:A:240:THR:C	2.39	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:493:HIS:O	1:A:497:VAL:HG23	1.96	0.66
1:A:620:VAL:O	1:A:624:PHE:CD1	2.49	0.66
1:A:694:ARG:HG2	1:A:699:LEU:CD1	2.26	0.66
1:A:700:GLU:OE2	1:A:703:ARG:NH1	2.29	0.66
1:A:832:PHE:HE2	2:B:77:LYS:HZ3	1.41	0.66
1:A:836:LYS:HG2	1:A:839:LEU:CG	2.26	0.66
2:B:131:PRO:HB3	2:B:141:LYS:HD3	1.77	0.66
1:A:351:LEU:HD21	1:A:355:LYS:HE3	1.78	0.65
2:B:7:ARG:C	2:B:9:LYS:H	2.02	0.65
2:B:29:ARG:NH2	2:B:35:MET:H	1.94	0.65
1:A:230:VAL:HG12	1:A:441:LEU:HD21	1.78	0.65
1:A:826:TRP:O	1:A:827:GLU:C	2.39	0.65
2:B:131:PRO:HB3	2:B:141:LYS:HE2	1.78	0.65
1:A:88:MET:HE3	1:A:102:ASN:CB	2.25	0.65
1:A:440:TRP:CD1	1:A:621:LYS:HD2	2.32	0.65
1:A:360:ILE:HA	1:A:363:LEU:HD12	1.78	0.65
2:B:131:PRO:HB2	2:B:138:ASN:HB3	1.77	0.65
3:C:2:GLN:O	3:C:3:LEU:C	2.37	0.65
1:A:278:THR:HG22	1:A:316:PHE:HD2	1.60	0.65
2:B:101:PHE:CD2	2:B:139:TYR:CD2	2.84	0.65
2:B:115:GLY:O	3:C:23:GLY:HA2	1.97	0.65
1:A:160:TYR:OH	1:A:260:GLY:O	2.14	0.65
1:A:308:VAL:O	1:A:310:ASP:N	2.30	0.65
1:A:324:VAL:O	1:A:327:ILE:HG22	1.97	0.65
1:A:572:LYS:HB3	1:A:575:CYS:CB	2.21	0.65
1:A:756:ARG:HG2	1:A:756:ARG:HH11	1.61	0.65
1:A:826:TRP:CD1	2:B:76:GLU:OE2	2.50	0.65
2:B:123:ILE:CG2	2:B:127:TRP:HE1	2.10	0.65
2:B:124:LYS:C	2:B:126:VAL:H	2.05	0.65
1:A:141:ARG:NH2	1:A:199:SER:CB	2.46	0.65
3:C:3:LEU:HD21	3:C:73:GLU:CB	2.27	0.65
1:A:152:LEU:HD22	1:A:185:ASN:OD1	1.97	0.64
1:A:237:ALA:HB2	1:A:287:TYR:HA	1.78	0.64
1:A:400:CYS:C	1:A:404:PRO:HD3	2.22	0.64
1:A:487:LEU:CD2	1:A:659:MET:HE1	2.27	0.64
1:A:574:GLY:O	1:A:576:ALA:N	2.30	0.64
1:A:711:ASN:C	1:A:712:ARG:HG3	2.21	0.64
1:A:820:TRP:O	1:A:824:ARG:HG2	1.96	0.64
1:A:85:ASN:HD22	1:A:86:MET:H	1.43	0.64
1:A:400:CYS:CA	1:A:404:PRO:HD3	2.25	0.64
3:C:88:MET:HE3	3:C:142:TYR:CE1	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:PHE:HD1	1:A:364:GLY:HA3	1.60	0.64
3:C:29:ASP:OD2	3:C:58:MET:O	2.16	0.64
1:A:196:VAL:O	1:A:199:SER:CB	2.45	0.64
1:A:316:PHE:CD1	1:A:364:GLY:CA	2.80	0.64
1:A:290:PHE:CD1	1:A:317:ILE:HD11	2.33	0.64
1:A:617:GLU:C	1:A:620:VAL:HG23	2.23	0.64
1:A:830:ARG:O	1:A:834:LYS:HG3	1.98	0.64
1:A:15:LEU:HD22	1:A:84:MET:HG3	1.80	0.64
1:A:618:PRO:C	1:A:620:VAL:H	2.04	0.64
2:B:26:ASP:OD1	2:B:28:ASP:OD2	2.14	0.64
1:A:64:GLN:O	1:A:65:GLU:HB2	1.98	0.64
1:A:403:LYS:O	1:A:415:GLN:HA	1.98	0.64
2:B:131:PRO:HD2	2:B:137:PHE:CE1	2.33	0.64
1:A:289:ILE:HA	1:A:292:GLN:HB2	1.79	0.64
1:A:551:LYS:CG	1:A:555:TYR:HE1	2.11	0.64
2:B:150:GLU:CG	2:B:151:ASP:H	2.09	0.64
1:A:2:THR:CG2	1:A:143:LYS:NZ	2.59	0.63
1:A:285:ARG:HH21	1:A:291:TYR:CB	2.11	0.63
2:B:81:THR:O	2:B:81:THR:CG2	2.46	0.63
1:A:3:MET:SD	1:A:149:PRO:HG3	2.38	0.63
1:A:551:LYS:HG2	1:A:555:TYR:HE1	1.62	0.63
2:B:35:MET:CE	2:B:54:LEU:HD23	2.27	0.63
1:A:6:SER:O	1:A:8:PRO:N	2.31	0.63
1:A:86:MET:CE	1:A:149:PRO:HA	2.28	0.63
1:A:620:VAL:O	1:A:624:PHE:HD1	1.82	0.63
1:A:839:LEU:HD13	2:B:20:GLU:HB3	1.79	0.63
3:C:119:THR:HG22	3:C:121:ASP:N	2.14	0.63
1:A:800:TYR:CE2	1:A:804:GLN:NE2	2.67	0.63
1:A:802:LYS:HE2	1:A:806:GLN:HE21	1.61	0.63
1:A:816:ASN:HD21	2:B:82:ASP:HB2	1.63	0.63
1:A:525:LEU:HD23	1:A:582:LEU:HD22	1.80	0.63
1:A:611:LEU:C	1:A:613:GLN:H	2.07	0.63
2:B:27:GLN:HA	2:B:27:GLN:OE1	1.98	0.63
2:B:28:ASP:OD1	2:B:29:ARG:HG2	1.98	0.63
1:A:564:MET:HE2	1:A:564:MET:N	2.14	0.63
1:A:290:PHE:HB3	1:A:317:ILE:CD1	2.29	0.63
1:A:317:ILE:CD1	1:A:361:LEU:HD21	2.28	0.63
2:B:29:ARG:NH2	2:B:34:GLY:HA2	2.14	0.63
3:C:12:ARG:HG3	3:C:12:ARG:HH11	1.63	0.63
3:C:104:SER:HB3	3:C:140:ILE:CD1	2.29	0.63
1:A:230:VAL:CG1	1:A:441:LEU:HD11	2.28	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:119:THR:HG22	3:C:121:ASP:H	1.63	0.62
1:A:337:ASP:O	1:A:341:ASP:OD1	2.17	0.62
1:A:826:TRP:CH2	2:B:60:GLU:CD	2.77	0.62
2:B:147:GLY:O	2:B:148:LYS:HG3	1.99	0.62
3:C:80:THR:O	3:C:80:THR:HG23	1.98	0.62
1:A:84:MET:CE	1:A:105:SER:HB2	2.23	0.62
1:A:540:CYS:O	1:A:601:LYS:HE2	1.98	0.62
3:C:67:GLU:C	3:C:70:PRO:HD2	2.25	0.62
1:A:3:MET:SD	1:A:149:PRO:CG	2.88	0.62
1:A:248:PHE:HE2	1:A:250:LYS:HB3	1.64	0.62
3:C:4:THR:H	3:C:7:GLU:HG3	1.65	0.62
1:A:181:GLY:C	1:A:183:THR:N	2.51	0.62
1:A:285:ARG:HG2	1:A:291:TYR:CE1	2.34	0.62
1:A:831:LEU:O	1:A:835:VAL:N	2.31	0.62
1:A:78:ASN:OD1	1:A:93:PHE:CB	2.45	0.62
1:A:82:PHE:O	1:A:85:ASN:HB2	2.00	0.62
1:A:392:VAL:HG11	1:A:611:LEU:HG	1.82	0.62
2:B:26:ASP:O	2:B:27:GLN:HB2	1.98	0.62
2:B:51:ASP:O	2:B:52:ASP:C	2.42	0.62
1:A:167:ARG:NH2	1:A:258:THR:HG23	2.13	0.62
1:A:820:TRP:CE3	1:A:821:LEU:HD23	2.34	0.62
2:B:150:GLU:HG2	2:B:151:ASP:H	1.65	0.62
1:A:7:ASP:O	1:A:9:ASP:N	2.33	0.62
1:A:51:THR:HG22	1:A:52:LYS:H	1.64	0.62
1:A:344:GLY:O	1:A:345:PHE:CD2	2.53	0.62
1:A:440:TRP:CD1	1:A:621:LYS:HZ2	2.18	0.62
1:A:200:LEU:HD11	1:A:259:GLN:O	1.99	0.61
1:A:321:THR:HG22	1:A:322:LEU:N	2.15	0.61
1:A:750:LEU:CD1	1:A:771:MET:HE1	2.28	0.61
1:A:3:MET:CE	1:A:14:CYS:SG	2.87	0.61
1:A:693:LEU:HA	1:A:696:ASN:HD22	1.65	0.61
2:B:29:ARG:NE	2:B:34:GLY:HA3	2.15	0.61
2:B:41:MET:C	2:B:43:SER:H	2.07	0.61
1:A:35:TRP:HH2	1:A:101:HIS:ND1	1.98	0.61
2:B:12:GLN:CD	2:B:13:ARG:HH12	2.08	0.61
1:A:142:GLY:HA2	1:A:161:GLN:NE2	2.15	0.61
1:A:579:HIS:ND1	1:A:593:ILE:HB	2.15	0.61
2:B:84:GLU:CG	2:B:85:ASP:H	1.97	0.61
3:C:70:PRO:O	3:C:74:GLU:HG2	1.99	0.61
1:A:3:MET:CE	1:A:10:MET:SD	2.88	0.61
1:A:226:GLN:O	1:A:229:PRO:HD2	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:112:GLU:HG3	2:B:123:ILE:HD11	1.83	0.61
2:B:7:ARG:O	2:B:9:LYS:N	2.33	0.61
2:B:133:LYS:O	2:B:135:LYS:N	2.34	0.61
1:A:191:GLN:HA	1:A:221:GLU:OE2	2.00	0.61
1:A:300:GLU:HG3	1:A:301:ASN:H	1.65	0.61
1:A:413:VAL:CG1	1:A:413:VAL:O	2.49	0.61
1:A:450:ASP:OD1	1:A:452:LYS:HG2	2.00	0.61
1:A:802:LYS:HE2	1:A:806:GLN:HE22	1.60	0.61
1:A:257:GLY:HA3	1:A:261:LYS:HE3	1.83	0.61
2:B:131:PRO:O	2:B:132:LEU:HD23	2.01	0.61
1:A:800:TYR:O	1:A:804:GLN:HG3	2.00	0.61
1:A:58:VAL:HG12	1:A:59:LYS:N	2.16	0.61
1:A:234:TYR:OH	1:A:353:MET:HG3	2.01	0.61
1:A:365:GLU:O	1:A:367:LYS:N	2.34	0.60
1:A:141:ARG:HH11	1:A:141:ARG:HG2	1.67	0.60
2:B:84:GLU:HG3	2:B:85:ASP:N	2.05	0.60
1:A:290:PHE:HB3	1:A:317:ILE:HD11	1.83	0.60
1:A:31:LYS:C	1:A:32:LYS:HG2	2.26	0.60
1:A:200:LEU:O	1:A:202:GLY:N	2.34	0.60
3:C:134:GLU:HA	3:C:139:ASN:O	2.00	0.60
1:A:157:ASP:OD1	1:A:161:GLN:NE2	2.34	0.60
1:A:487:LEU:HD23	1:A:659:MET:HE1	1.83	0.60
3:C:67:GLU:O	3:C:70:PRO:HD2	2.02	0.60
1:A:239:THR:O	1:A:241:ARG:N	2.34	0.60
1:A:305:ILE:O	1:A:306:LEU:HG	2.02	0.60
2:B:7:ARG:O	2:B:8:VAL:C	2.44	0.60
1:A:383:ALA:HA	1:A:386:VAL:HG22	1.84	0.60
1:A:413:VAL:C	1:A:415:GLN:H	2.10	0.60
1:A:811:THR:O	1:A:815:ARG:HB3	2.02	0.60
1:A:196:VAL:HA	1:A:199:SER:OG	2.02	0.59
1:A:828:TRP:CD1	2:B:60:GLU:OE1	2.55	0.59
1:A:839:LEU:HD13	2:B:20:GLU:CB	2.32	0.59
1:A:184:GLU:O	1:A:187:LYS:HB3	2.01	0.59
1:A:620:VAL:O	1:A:624:PHE:CB	2.43	0.59
1:A:786:MET:O	1:A:789:ALA:HB3	2.02	0.59
1:A:450:ASP:OD1	1:A:450:ASP:O	2.21	0.59
1:A:85:ASN:ND2	1:A:86:MET:N	2.50	0.59
1:A:819:LYS:HE2	2:B:79:SER:HB2	1.85	0.59
2:B:101:PHE:CD1	2:B:138:ASN:HA	2.37	0.59
3:C:36:LEU:CD2	3:C:68:ILE:HD13	2.33	0.59
1:A:836:LYS:O	1:A:837:PRO:C	2.45	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:ASP:OD1	1:A:350:LYS:HE3	2.02	0.59
1:A:290:PHE:CG	1:A:317:ILE:HD11	2.38	0.59
1:A:756:ARG:HG2	1:A:756:ARG:NH1	2.15	0.59
3:C:30:ALA:HA	3:C:33:VAL:HG23	1.84	0.59
1:A:617:GLU:HA	1:A:620:VAL:CG2	2.32	0.59
1:A:693:LEU:HB3	1:A:699:LEU:HG	1.84	0.59
2:B:41:MET:C	2:B:43:SER:N	2.60	0.59
3:C:104:SER:HB3	3:C:140:ILE:HG13	1.85	0.59
1:A:830:ARG:O	1:A:833:ASN:HB2	2.03	0.58
2:B:32:PHE:CE2	2:B:64:GLN:HG2	2.37	0.58
1:A:120:CYS:HB2	1:A:155:ILE:CD1	2.32	0.58
1:A:280:GLN:HB2	1:A:320:GLY:N	2.18	0.58
1:A:86:MET:CE	1:A:150:PRO:HD3	2.33	0.58
1:A:820:TRP:HE1	2:B:145:ILE:HG22	1.68	0.58
2:B:94:PHE:O	2:B:102:ILE:HG12	2.03	0.58
1:A:298:PHE:N	1:A:299:PRO:CD	2.67	0.58
1:A:413:VAL:O	1:A:413:VAL:HG12	2.03	0.58
1:A:547:ASP:OD2	1:A:594:ALA:HA	2.02	0.58
1:A:836:LYS:C	1:A:838:LEU:N	2.56	0.58
2:B:10:LEU:HB2	2:B:78:VAL:CG2	2.33	0.58
1:A:4:ASP:C	1:A:6:SER:N	2.55	0.58
1:A:191:GLN:CG	1:A:221:GLU:HG2	2.13	0.58
1:A:130:PRO:O	1:A:132:TYR:N	2.37	0.58
1:A:136:LEU:O	1:A:139:LYS:N	2.35	0.58
1:A:4:ASP:O	1:A:6:SER:N	2.35	0.58
1:A:278:THR:CG2	1:A:316:PHE:CE2	2.86	0.57
2:B:56:ALA:O	2:B:59:LYS:HG3	2.04	0.57
1:A:728:ASN:OD1	1:A:728:ASN:C	2.47	0.57
1:A:186:THR:HG23	1:A:461:VAL:HG11	1.84	0.57
1:A:54:ASP:HA	1:A:71:LYS:HD2	1.85	0.57
1:A:86:MET:HE3	1:A:150:PRO:HD3	1.86	0.57
1:A:393:ASN:O	1:A:396:ASP:N	2.37	0.57
1:A:608:VAL:O	1:A:612:LEU:CG	2.49	0.57
1:A:823:LEU:O	1:A:829:TRP:CD1	2.57	0.57
2:B:94:PHE:CD2	2:B:110:LEU:HD21	2.40	0.57
3:C:57:LYS:HG3	3:C:60:GLU:HG3	1.86	0.57
1:A:293:LEU:N	1:A:333:MET:HE3	2.20	0.57
1:A:391:GLY:HA3	1:A:616:LYS:HG2	1.86	0.57
1:A:85:ASN:HD22	1:A:86:MET:N	2.01	0.57
1:A:88:MET:HE1	1:A:99:ILE:CA	2.34	0.57
1:A:157:ASP:O	1:A:161:GLN:HG3	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:ARG:CZ	1:A:199:SER:CB	2.82	0.57
1:A:346:THR:C	1:A:348:GLU:N	2.61	0.57
1:A:533:LEU:O	1:A:537:GLU:HG3	2.05	0.57
1:A:831:LEU:C	1:A:833:ASN:H	2.13	0.57
1:A:279:TYR:HA	1:A:319:GLN:OE1	2.05	0.57
1:A:348:GLU:HA	1:A:348:GLU:OE1	2.04	0.57
1:A:555:TYR:HD2	1:A:559:LEU:HD11	1.71	0.56
2:B:143:VAL:O	2:B:146:LYS:HB2	2.05	0.56
3:C:15:PHE:CG	3:C:65:LEU:HD13	2.40	0.56
2:B:85:ASP:O	2:B:86:ALA:C	2.49	0.56
1:A:41:PHE:CD2	1:A:41:PHE:N	2.72	0.56
1:A:184:GLU:HG3	1:A:185:ASN:N	2.19	0.56
1:A:383:ALA:HA	1:A:386:VAL:CG2	2.35	0.56
2:B:22:PHE:HA	2:B:33:ILE:HD11	1.87	0.56
1:A:417:ARG:HA	1:A:421:GLN:OE1	2.06	0.56
1:A:644:PHE:N	1:A:644:PHE:HD1	2.04	0.56
1:A:836:LYS:HG2	1:A:839:LEU:HD11	1.87	0.56
3:C:132:ILE:HD12	3:C:145:LEU:HD13	1.88	0.56
1:A:88:MET:CE	1:A:99:ILE:HG23	2.35	0.56
1:A:128:ARG:HG2	1:A:128:ARG:HH11	1.71	0.56
1:A:836:LYS:HG2	1:A:839:LEU:HG	1.88	0.56
2:B:28:ASP:OD1	2:B:37:ASP:OD2	2.24	0.56
1:A:328:ASP:O	1:A:329:ASP:C	2.49	0.56
1:A:555:TYR:O	1:A:556:ASP:C	2.49	0.56
3:C:141:LYS:HB2	3:C:144:ASP:HB2	1.86	0.56
1:A:88:MET:HE1	1:A:99:ILE:O	2.06	0.56
1:A:672:CYS:C	1:A:673:ILE:HG13	2.31	0.56
1:A:713:ILE:HG22	1:A:714:ILE:O	2.06	0.56
3:C:102:ILE:HG22	3:C:103:SER:O	2.06	0.56
2:B:50:PRO:HG2	2:B:53:GLU:OE1	2.06	0.55
3:C:4:THR:O	3:C:8:ILE:HG13	2.06	0.55
1:A:35:TRP:CH2	1:A:101:HIS:ND1	2.75	0.55
1:A:302:ILE:HG21	1:A:309:PRO:HD3	1.88	0.55
1:A:305:ILE:HG23	1:A:358:GLY:HA3	1.88	0.55
1:A:87:ASP:HA	1:A:115:TYR:O	2.06	0.55
3:C:78:LYS:CE	3:C:79:ASP:H	2.19	0.55
1:A:4:ASP:OD1	1:A:6:SER:HB2	2.05	0.55
1:A:620:VAL:HG12	1:A:624:PHE:CD1	2.41	0.55
1:A:836:LYS:HD3	2:B:17:GLU:O	2.06	0.55
1:A:139:LYS:O	1:A:148:MET:SD	2.64	0.55
1:A:236:ASN:HB3	1:A:244:ASN:HD21	1.69	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:644:PHE:N	1:A:644:PHE:CD1	2.75	0.55
2:B:132:LEU:O	2:B:133:LYS:CG	2.55	0.55
1:A:357:THR:OG1	1:A:437:MET:HE1	2.07	0.55
1:A:396:ASP:O	1:A:400:CYS:SG	2.65	0.55
1:A:406:ILE:CG2	1:A:407:LYS:N	2.65	0.55
3:C:126:ILE:HD11	3:C:149:VAL:HG22	1.88	0.55
1:A:278:THR:CG2	1:A:316:PHE:HE2	2.20	0.55
2:B:145:ILE:O	2:B:146:LYS:C	2.48	0.55
1:A:63:THR:O	1:A:64:GLN:HB2	2.06	0.55
1:A:85:ASN:ND2	1:A:86:MET:H	2.05	0.55
1:A:191:GLN:O	1:A:194:ALA:HB3	2.06	0.55
1:A:352:SER:CB	1:A:618:PRO:HG3	2.37	0.55
2:B:22:PHE:CD1	2:B:22:PHE:C	2.84	0.55
3:C:78:LYS:HG3	3:C:79:ASP:N	2.22	0.55
3:C:132:ILE:HD13	3:C:145:LEU:HA	1.88	0.55
1:A:35:TRP:CE2	1:A:77:ARG:HG3	2.42	0.55
1:A:54:ASP:HA	1:A:71:LYS:CD	2.37	0.55
1:A:618:PRO:C	1:A:620:VAL:N	2.65	0.55
2:B:74:PHE:CE2	2:B:77:LYS:NZ	2.75	0.55
3:C:4:THR:CB	3:C:7:GLU:HG3	2.37	0.55
1:A:107:TYR:OH	1:A:124:ASN:O	2.19	0.55
1:A:346:THR:C	1:A:348:GLU:H	2.14	0.55
1:A:488:GLN:OE1	1:A:697:GLY:HA3	2.07	0.55
1:A:571:PRO:HD2	1:A:575:CYS:O	2.07	0.55
1:A:820:TRP:CZ3	1:A:821:LEU:HD23	2.41	0.55
1:A:156:ALA:HB1	1:A:193:PHE:CE1	2.42	0.54
1:A:678:LEU:O	1:A:680:THR:N	2.40	0.54
3:C:93:THR:HG23	3:C:94:PHE:CD1	2.41	0.54
1:A:491:PHE:O	1:A:492:ASN:C	2.50	0.54
1:A:832:PHE:HA	1:A:835:VAL:HB	1.90	0.54
2:B:85:ASP:O	2:B:88:ARG:N	2.40	0.54
3:C:117:ARG:HH11	3:C:117:ARG:CG	2.20	0.54
3:C:132:ILE:HD13	3:C:145:LEU:CA	2.37	0.54
1:A:132:TYR:CE2	1:A:188:LYS:HD3	2.43	0.54
1:A:440:TRP:CG	1:A:621:LYS:HZ2	2.24	0.54
1:A:831:LEU:HD11	2:B:57:MET:HE1	1.90	0.54
1:A:68:VAL:HG12	1:A:68:VAL:O	2.06	0.54
1:A:248:PHE:CE2	1:A:250:LYS:HB3	2.42	0.54
1:A:818:ARG:HH21	2:B:118:PHE:HD1	1.56	0.54
2:B:14:GLN:HE22	2:B:81:THR:CG2	2.20	0.54
1:A:402:LEU:C	1:A:403:LYS:HG2	2.33	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:29:ARG:NH2	2:B:34:GLY:HA3	2.23	0.54
3:C:102:ILE:HG13	3:C:142:TYR:HD2	1.71	0.54
1:A:126:TYR:O	1:A:127:ARG:HB3	2.07	0.54
1:A:332:GLU:C	1:A:334:GLY:N	2.60	0.54
1:A:296:PRO:HA	1:A:299:PRO:HD3	1.89	0.54
1:A:413:VAL:CG1	1:A:415:GLN:HB2	2.22	0.54
1:A:155:ILE:O	1:A:155:ILE:CG2	2.56	0.54
1:A:579:HIS:O	1:A:580:PHE:HB3	2.07	0.54
1:A:746:SER:O	1:A:749:GLN:N	2.29	0.54
1:A:820:TRP:HB3	2:B:146:LYS:NZ	2.23	0.54
3:C:132:ILE:HD12	3:C:145:LEU:CD1	2.37	0.54
1:A:259:GLN:H	1:A:261:LYS:CE	2.03	0.54
1:A:727:PRO:HG3	3:C:86:GLU:HG2	1.90	0.54
1:A:820:TRP:NE1	2:B:145:ILE:HG22	2.23	0.54
3:C:130:CYS:O	3:C:148:LYS:CD	2.53	0.54
1:A:74:ILE:HG13	1:A:74:ILE:O	2.07	0.53
2:B:147:GLY:O	2:B:148:LYS:CB	2.56	0.53
2:B:32:PHE:CZ	2:B:64:GLN:NE2	2.76	0.53
2:B:120:LYS:CA	2:B:123:ILE:HD12	2.29	0.53
3:C:74:GLU:O	3:C:77:SER:HB2	2.08	0.53
1:A:352:SER:HB3	1:A:618:PRO:HG3	1.89	0.53
2:B:32:PHE:CE2	2:B:64:GLN:NE2	2.75	0.53
2:B:98:GLY:O	2:B:99:GLN:O	2.25	0.53
1:A:58:VAL:CG1	1:A:59:LYS:N	2.72	0.53
1:A:406:ILE:HG13	1:A:414:THR:HG21	1.91	0.53
3:C:4:THR:N	3:C:7:GLU:HG3	2.22	0.53
1:A:182:LYS:N	4:A:1001:SO4:O1	2.41	0.53
1:A:305:ILE:O	1:A:306:LEU:CB	2.57	0.53
1:A:313:LEU:HD23	1:A:313:LEU:N	2.18	0.53
1:A:400:CYS:SG	1:A:611:LEU:HD22	2.48	0.53
1:A:518:ASP:C	1:A:519:LEU:HD23	2.34	0.53
1:A:827:GLU:OE1	1:A:830:ARG:CZ	2.57	0.53
2:B:88:ARG:HD3	2:B:140:ASN:OD1	2.08	0.53
1:A:183:THR:O	1:A:184:GLU:C	2.51	0.53
2:B:48:VAL:HG12	2:B:48:VAL:O	2.07	0.53
1:A:36:VAL:HG21	1:A:69:VAL:HG21	1.91	0.53
1:A:572:LYS:C	1:A:574:GLY:H	2.17	0.53
3:C:117:ARG:HG3	3:C:117:ARG:NH1	2.23	0.53
1:A:141:ARG:HG2	1:A:141:ARG:NH1	2.24	0.53
1:A:329:ASP:O	1:A:332:GLU:N	2.42	0.53
1:A:368:TRP:CE3	1:A:377:ALA:HA	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:22:PHE:CE2	2:B:66:ASN:O	2.62	0.53
2:B:66:ASN:OD1	2:B:66:ASN:N	2.35	0.53
1:A:127:ARG:NE	1:A:129:LEU:HD21	2.24	0.53
1:A:140:TYR:CE1	1:A:148:MET:HE2	2.45	0.53
1:A:352:SER:O	1:A:353:MET:C	2.51	0.53
1:A:128:ARG:HG2	1:A:128:ARG:NH1	2.23	0.52
1:A:611:LEU:C	1:A:613:GLN:N	2.65	0.52
2:B:41:MET:O	2:B:43:SER:N	2.42	0.52
3:C:78:LYS:HE3	3:C:78:LYS:CA	2.36	0.52
1:A:617:GLU:HA	1:A:620:VAL:HG23	1.91	0.52
1:A:762:VAL:HG13	1:A:762:VAL:O	2.10	0.52
2:B:13:ARG:O	2:B:17:GLU:HB2	2.09	0.52
1:A:367:LYS:NZ	1:A:382:GLU:CD	2.67	0.52
1:A:820:TRP:CG	2:B:146:LYS:HZ2	2.27	0.52
2:B:29:ARG:NH2	2:B:35:MET:N	2.57	0.52
2:B:94:PHE:CD1	2:B:94:PHE:N	2.77	0.52
1:A:467:PHE:HB3	1:A:695:CYS:HB3	1.91	0.52
1:A:820:TRP:HB3	2:B:146:LYS:HZ1	1.74	0.52
2:B:58:LEU:O	2:B:60:GLU:N	2.42	0.52
1:A:236:ASN:HD22	1:A:244:ASN:ND2	2.07	0.52
1:A:298:PHE:H	1:A:299:PRO:HD3	1.73	0.52
1:A:346:THR:HG22	1:A:348:GLU:CB	2.39	0.52
1:A:826:TRP:HB3	1:A:829:TRP:HB2	1.92	0.52
2:B:32:PHE:O	2:B:34:GLY:N	2.43	0.52
3:C:4:THR:HG23	3:C:7:GLU:CD	2.34	0.52
1:A:383:ALA:O	1:A:386:VAL:HG23	2.09	0.52
1:A:713:ILE:CD1	1:A:769:LEU:HD21	2.39	0.52
1:A:794:TYR:CZ	3:C:153:PRO:HA	2.44	0.52
1:A:365:GLU:HB3	1:A:367:LYS:NZ	2.25	0.52
2:B:114:MET:HE2	3:C:21:TRP:CE3	2.44	0.52
2:B:132:LEU:HD21	2:B:137:PHE:HD1	1.75	0.52
3:C:104:SER:O	3:C:108:ARG:HG3	2.10	0.52
3:C:153:PRO:C	3:C:155:PRO:HD3	2.34	0.52
1:A:51:THR:CG2	1:A:52:LYS:H	2.23	0.52
1:A:616:LYS:H	1:A:616:LYS:HD3	1.74	0.52
1:A:690:LEU:O	1:A:691:HIS:C	2.51	0.52
2:B:47:ARG:O	2:B:48:VAL:CB	2.58	0.52
2:B:67:PHE:CE1	2:B:71:LEU:HD21	2.45	0.52
2:B:127:TRP:O	2:B:128:LYS:C	2.53	0.52
2:B:145:ILE:O	2:B:148:LYS:CG	2.58	0.52
1:A:14:CYS:O	1:A:15:LEU:CB	2.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:GLU:HB2	1:A:188:LYS:HE3	1.92	0.52
1:A:836:LYS:HD2	2:B:17:GLU:OE2	2.09	0.52
2:B:14:GLN:NE2	2:B:81:THR:HG23	2.24	0.52
2:B:34:GLY:O	2:B:38:LEU:N	2.40	0.52
1:A:76:GLN:OE1	1:A:93:PHE:CE2	2.63	0.52
1:A:285:ARG:NH2	1:A:291:TYR:HB2	2.25	0.52
1:A:363:LEU:HD22	1:A:429:LEU:HD23	1.92	0.52
1:A:703:ARG:O	1:A:706:ARG:HB2	2.10	0.52
1:A:728:ASN:C	3:C:85:ASP:CG	2.78	0.52
2:B:132:LEU:CD2	2:B:137:PHE:HD1	2.22	0.52
1:A:88:MET:HA	1:A:91:LEU:HG	1.91	0.51
1:A:178:SER:O	4:A:1001:SO4:S	2.68	0.51
1:A:374:GLN:CD	1:A:415:GLN:NE2	2.67	0.51
1:A:390:LEU:O	1:A:619:ILE:HD12	2.09	0.51
1:A:688:LEU:O	1:A:692:GLN:HG3	2.10	0.51
1:A:809:GLY:O	1:A:812:LEU:N	2.43	0.51
1:A:836:LYS:HG2	1:A:839:LEU:CD1	2.40	0.51
1:A:179:GLY:O	1:A:674:ILE:HG12	2.11	0.51
1:A:321:THR:CG2	1:A:322:LEU:N	2.73	0.51
1:A:490:PHE:HD1	1:A:663:TYR:CE2	2.29	0.51
1:A:618:PRO:O	1:A:620:VAL:N	2.43	0.51
1:A:751:ASP:HB3	1:A:754:GLU:HG2	1.92	0.51
2:B:13:ARG:N	2:B:13:ARG:CD	2.73	0.51
2:B:53:GLU:O	2:B:55:ASN:N	2.43	0.51
1:A:483:THR:HA	1:A:655:LEU:HD21	1.93	0.51
3:C:118:ILE:HG23	3:C:122:GLN:HB2	1.92	0.51
1:A:274:LYS:O	1:A:276:ARG:N	2.44	0.51
1:A:390:LEU:HD22	1:A:619:ILE:CD1	2.39	0.51
1:A:514:ASP:OD1	1:A:516:GLY:N	2.40	0.51
2:B:47:ARG:O	2:B:48:VAL:HB	2.10	0.51
1:A:293:LEU:HD13	1:A:305:ILE:CD1	2.41	0.51
1:A:348:GLU:O	1:A:349:GLU:C	2.53	0.51
1:A:547:ASP:CG	1:A:595:GLY:H	2.18	0.51
1:A:831:LEU:C	1:A:833:ASN:N	2.68	0.51
2:B:89:ASN:O	2:B:92:SER:HB2	2.10	0.51
3:C:73:GLU:HA	3:C:76:SER:OG	2.10	0.51
1:A:107:TYR:CD2	1:A:684:ILE:HD11	2.46	0.51
1:A:178:SER:O	4:A:1001:SO4:O3	2.28	0.51
1:A:230:VAL:CG1	1:A:441:LEU:HD21	2.40	0.51
1:A:346:THR:HB	1:A:349:GLU:CG	2.41	0.51
1:A:417:ARG:NE	1:A:417:ARG:N	2.49	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:499:GLU:OE1	1:A:712:ARG:NH2	2.33	0.51
1:A:620:VAL:HG12	1:A:624:PHE:HE1	1.75	0.51
2:B:42:PHE:HA	2:B:45:LEU:HB2	1.92	0.51
1:A:180:ALA:HB1	1:A:672:CYS:HB3	1.93	0.51
1:A:413:VAL:C	1:A:415:GLN:N	2.68	0.51
2:B:147:GLY:O	2:B:148:LYS:HB2	2.09	0.51
3:C:30:ALA:CB	3:C:55:THR:HG23	2.40	0.51
1:A:140:TYR:CZ	1:A:148:MET:HE2	2.46	0.51
1:A:351:LEU:HD11	1:A:355:LYS:HE3	1.91	0.51
1:A:365:GLU:O	1:A:366:MET:C	2.54	0.51
1:A:513:ILE:O	1:A:514:ASP:C	2.53	0.51
2:B:34:GLY:N	2:B:37:ASP:HB2	2.21	0.51
2:B:13:ARG:HD2	2:B:13:ARG:H	1.74	0.51
2:B:145:ILE:O	2:B:148:LYS:HG3	2.11	0.51
1:A:36:VAL:HG22	1:A:69:VAL:HG21	1.94	0.50
1:A:51:THR:CG2	1:A:52:LYS:N	2.74	0.50
1:A:546:SER:N	1:A:549:SER:OG	2.43	0.50
2:B:142:MET:HE1	2:B:146:LYS:CD	2.26	0.50
1:A:568:PRO:CG	1:A:578:ALA:HB3	2.40	0.50
1:A:307:ALA:HB1	1:A:314:TYR:OH	2.11	0.50
1:A:645:GLN:HA	1:A:645:GLN:OE1	2.10	0.50
2:B:12:GLN:CD	2:B:13:ARG:NH1	2.69	0.50
2:B:67:PHE:HA	2:B:70:PHE:CB	2.41	0.50
1:A:46:ALA:HB1	1:A:58:VAL:CG1	2.41	0.50
1:A:308:VAL:O	1:A:308:VAL:HG23	2.12	0.50
1:A:440:TRP:CD1	1:A:621:LYS:CD	2.94	0.50
1:A:324:VAL:O	1:A:327:ILE:CG2	2.60	0.50
1:A:794:TYR:CD1	3:C:153:PRO:HD3	2.47	0.50
1:A:363:LEU:HD23	1:A:366:MET:SD	2.52	0.50
1:A:369:LYS:CD	1:A:370:GLN:H	2.25	0.50
1:A:36:VAL:HG22	1:A:37:PRO:HD2	1.93	0.50
1:A:351:LEU:HD21	1:A:355:LYS:CE	2.42	0.49
1:A:643:ALA:O	1:A:644:PHE:O	2.30	0.49
1:A:715:TYR:CE1	1:A:738:LYS:HG3	2.47	0.49
1:A:820:TRP:CB	2:B:146:LYS:NZ	2.75	0.49
1:A:63:THR:C	1:A:64:GLN:O	2.53	0.49
1:A:403:LYS:O	1:A:415:GLN:CA	2.60	0.49
1:A:510:TRP:CZ2	1:A:512:PHE:HB2	2.46	0.49
1:A:793:GLY:O	1:A:797:ARG:HB2	2.12	0.49
3:C:42:MET:HE1	3:C:75:MET:HG3	1.94	0.49
1:A:304:LYS:HB3	1:A:355:LYS:HE2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:THR:HB	1:A:349:GLU:HG3	1.94	0.49
1:A:832:PHE:CE2	2:B:77:LYS:HD3	2.47	0.49
1:A:86:MET:HE3	1:A:149:PRO:HB3	1.94	0.49
1:A:571:PRO:HB2	1:A:575:CYS:SG	2.53	0.49
1:A:800:TYR:CE1	3:C:17:LEU:HD22	2.47	0.49
2:B:12:GLN:HB3	2:B:13:ARG:NH1	2.27	0.49
1:A:249:GLY:HA3	1:A:464:ILE:HD12	1.93	0.49
1:A:443:ARG:HH12	1:A:621:LYS:HD2	1.77	0.49
2:B:114:MET:HE2	3:C:21:TRP:HE3	1.77	0.49
1:A:354:TYR:O	1:A:357:THR:HB	2.11	0.49
1:A:832:PHE:HE2	2:B:77:LYS:NZ	2.07	0.49
3:C:14:VAL:CG1	3:C:36:LEU:HD12	2.43	0.49
1:A:678:LEU:O	1:A:679:LYS:C	2.55	0.49
2:B:33:ILE:HB	2:B:65:LEU:HD23	1.95	0.49
3:C:132:ILE:CD1	3:C:145:LEU:CA	2.89	0.49
1:A:153:PHE:CD2	1:A:192:TYR:CD2	3.01	0.49
1:A:564:MET:HE2	1:A:564:MET:H	1.76	0.49
1:A:569:LYS:O	1:A:570:PRO:O	2.30	0.49
2:B:53:GLU:O	2:B:54:LEU:C	2.56	0.49
1:A:329:ASP:O	1:A:330:GLU:C	2.55	0.49
1:A:602:ASP:OD1	1:A:602:ASP:O	2.31	0.49
1:A:698:VAL:HG12	1:A:699:LEU:N	2.27	0.49
2:B:28:ASP:CG	2:B:29:ARG:HG2	2.38	0.49
2:B:131:PRO:CB	2:B:141:LYS:HD3	2.42	0.49
3:C:135:ASP:OD1	3:C:136:ILE:N	2.46	0.49
1:A:178:SER:O	4:A:1001:SO4:O2	2.30	0.48
1:A:199:SER:C	1:A:200:LEU:HD23	2.37	0.48
1:A:15:LEU:CD2	1:A:84:MET:HG3	2.41	0.48
1:A:136:LEU:O	1:A:137:VAL:C	2.56	0.48
1:A:173:LEU:HD22	1:A:462:LEU:CD2	2.42	0.48
1:A:236:ASN:CB	1:A:244:ASN:HD21	2.26	0.48
1:A:600:ASN:ND2	1:A:648:SER:H	2.04	0.48
3:C:74:GLU:O	3:C:77:SER:N	2.33	0.48
1:A:133:THR:HG22	1:A:134:GLN:N	2.29	0.48
1:A:624:PHE:O	1:A:625:THR:C	2.57	0.48
1:A:659:MET:CE	1:A:662:LEU:HD12	2.43	0.48
1:A:181:GLY:O	1:A:182:LYS:C	2.57	0.48
1:A:479:CYS:HB3	1:A:651:HIS:CD2	2.49	0.48
1:A:617:GLU:HA	1:A:620:VAL:HG21	1.96	0.48
1:A:831:LEU:CD1	2:B:57:MET:HE1	2.44	0.48
2:B:28:ASP:OD1	2:B:37:ASP:CG	2.56	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:SER:O	1:A:8:PRO:CD	2.61	0.48
1:A:311:PRO:O	1:A:312:GLY:O	2.30	0.48
1:A:414:THR:C	1:A:416:GLY:H	2.21	0.48
1:A:115:TYR:CD1	1:A:150:PRO:HG3	2.49	0.48
1:A:193:PHE:CE2	1:A:459:ILE:HG21	2.49	0.48
1:A:298:PHE:HE1	1:A:333:MET:HG3	1.72	0.48
1:A:417:ARG:HE	1:A:417:ARG:CA	2.27	0.48
1:A:274:LYS:O	1:A:275:SER:C	2.57	0.48
1:A:374:GLN:NE2	1:A:415:GLN:HG2	2.28	0.48
1:A:487:LEU:HD21	1:A:659:MET:HE1	1.94	0.48
3:C:104:SER:HB3	3:C:140:ILE:CG1	2.44	0.48
1:A:71:LYS:O	1:A:74:ILE:HG12	2.14	0.48
1:A:136:LEU:CD2	1:A:139:LYS:HD2	2.42	0.48
1:A:713:ILE:O	1:A:761:LYS:HA	2.13	0.48
1:A:722:TYR:O	1:A:725:LEU:HB2	2.14	0.48
2:B:124:LYS:O	2:B:125:ASN:C	2.57	0.48
1:A:529:PRO:O	1:A:530:MET:HB2	2.14	0.48
1:A:669:PHE:N	1:A:669:PHE:CD1	2.82	0.48
3:C:12:ARG:HG3	3:C:12:ARG:NH1	2.27	0.48
1:A:406:ILE:O	1:A:407:LYS:HB3	2.13	0.48
2:B:7:ARG:O	2:B:78:VAL:CG1	2.44	0.48
2:B:35:MET:O	2:B:39:LYS:HG3	2.13	0.48
1:A:95:ASN:O	1:A:99:ILE:HG12	2.15	0.47
2:B:14:GLN:O	2:B:18:LEU:HG	2.14	0.47
2:B:55:ASN:O	2:B:58:LEU:HB2	2.14	0.47
2:B:133:LYS:O	2:B:134:ASN:C	2.57	0.47
3:C:16:ASP:HA	3:C:19:ASP:OD1	2.14	0.47
1:A:16:THR:OG1	1:A:19:LYS:HG3	2.15	0.47
1:A:163:MET:HE1	1:A:256:PHE:CG	2.50	0.47
1:A:193:PHE:HB3	1:A:256:PHE:HZ	1.79	0.47
1:A:227:CYS:HB3	1:A:445:VAL:HG11	1.96	0.47
1:A:345:PHE:CE2	1:A:444:ARG:NH2	2.64	0.47
1:A:388:PHE:O	1:A:391:GLY:N	2.47	0.47
1:A:406:ILE:HB	1:A:414:THR:CG2	2.44	0.47
2:B:29:ARG:O	2:B:30:ASP:C	2.57	0.47
1:A:3:MET:SD	1:A:149:PRO:HD3	2.55	0.47
1:A:84:MET:HE1	1:A:105:SER:CB	2.26	0.47
1:A:115:TYR:CZ	1:A:150:PRO:HA	2.49	0.47
2:B:67:PHE:C	2:B:70:PHE:H	2.21	0.47
3:C:14:VAL:HG12	3:C:36:LEU:CD1	2.45	0.47
3:C:102:ILE:O	3:C:103:SER:C	2.56	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:LYS:HE2	1:A:64:GLN:HE22	1.80	0.47
1:A:367:LYS:HD3	1:A:367:LYS:N	2.29	0.47
1:A:536:LEU:HD13	1:A:550:PHE:CZ	2.50	0.47
1:A:550:PHE:HE2	1:A:593:ILE:CD1	2.14	0.47
1:A:823:LEU:C	1:A:825:ASN:H	2.22	0.47
2:B:52:ASP:O	2:B:55:ASN:HB3	2.14	0.47
3:C:117:ARG:CG	3:C:117:ARG:NH1	2.76	0.47
1:A:563:PRO:CG	1:A:564:MET:HE2	2.43	0.47
2:B:8:VAL:HG23	2:B:9:LYS:HD2	1.97	0.47
2:B:119:SER:C	2:B:121:GLU:N	2.67	0.47
1:A:337:ASP:OD1	1:A:350:LYS:NZ	2.48	0.47
1:A:403:LYS:N	1:A:404:PRO:CD	2.67	0.47
1:A:539:GLU:OE2	1:A:549:SER:HB2	2.15	0.47
3:C:42:MET:CE	3:C:75:MET:HG3	2.44	0.47
1:A:88:MET:HE1	1:A:99:ILE:CG2	2.44	0.47
1:A:181:GLY:C	1:A:183:THR:H	2.22	0.47
1:A:337:ASP:OD1	1:A:350:LYS:CE	2.62	0.47
1:A:382:GLU:O	1:A:386:VAL:HG22	2.14	0.47
1:A:466:GLY:O	1:A:484:ASN:CG	2.57	0.47
1:A:603:PRO:CB	1:A:644:PHE:HB3	2.45	0.47
1:A:617:GLU:CA	1:A:620:VAL:HG23	2.45	0.47
2:B:10:LEU:HG	2:B:15:MET:HG2	1.97	0.47
3:C:14:VAL:HG21	3:C:40:LEU:HD23	1.96	0.47
1:A:99:ILE:HG13	1:A:702:ILE:HD13	1.97	0.47
1:A:192:TYR:CD1	1:A:192:TYR:C	2.93	0.47
1:A:692:GLN:O	1:A:696:ASN:ND2	2.47	0.47
2:B:10:LEU:HA	2:B:14:GLN:OE1	2.15	0.47
2:B:32:PHE:CD2	2:B:64:GLN:HG2	2.50	0.47
2:B:60:GLU:HB3	2:B:73:LEU:HD11	1.97	0.47
1:A:107:TYR:HA	1:A:111:PHE:O	2.15	0.47
1:A:170:GLN:O	1:A:459:ILE:HA	2.15	0.47
3:C:135:ASP:O	3:C:136:ILE:O	2.32	0.47
1:A:332:GLU:C	1:A:334:GLY:H	2.20	0.47
1:A:346:THR:HB	1:A:349:GLU:H	1.80	0.47
1:A:379:GLY:O	1:A:380:THR:OG1	2.19	0.47
1:A:551:LYS:O	1:A:555:TYR:HD1	1.97	0.47
2:B:29:ARG:O	2:B:32:PHE:HD1	1.98	0.47
1:A:160:TYR:OH	1:A:260:GLY:HA3	2.15	0.46
1:A:346:THR:HG22	1:A:348:GLU:HB3	1.96	0.46
1:A:351:LEU:O	1:A:355:LYS:N	2.41	0.46
1:A:358:GLY:O	1:A:361:LEU:HB2	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:368:TRP:CE3	1:A:402:LEU:HD21	2.50	0.46
1:A:386:VAL:HG23	1:A:387:ALA:N	2.29	0.46
1:A:727:PRO:HB2	3:C:85:ASP:HB3	1.96	0.46
1:A:836:LYS:HA	1:A:839:LEU:CD2	2.45	0.46
2:B:25:ILE:O	2:B:37:ASP:CB	2.53	0.46
2:B:142:MET:O	2:B:143:VAL:C	2.58	0.46
1:A:397:LEU:O	1:A:398:LEU:C	2.59	0.46
1:A:415:GLN:C	1:A:417:ARG:N	2.73	0.46
1:A:783:ILE:HG21	3:C:86:GLU:O	2.16	0.46
2:B:39:LYS:HE2	2:B:54:LEU:HD22	1.97	0.46
2:B:61:CYS:O	2:B:62:PRO:C	2.59	0.46
1:A:42:GLY:HA3	1:A:686:ALA:CB	2.45	0.46
1:A:115:TYR:CE1	1:A:150:PRO:HA	2.50	0.46
1:A:160:TYR:OH	1:A:260:GLY:CA	2.63	0.46
1:A:785:SER:HA	1:A:788:GLN:OE1	2.16	0.46
2:B:28:ASP:CG	2:B:37:ASP:OD2	2.58	0.46
3:C:35:ASP:O	3:C:36:LEU:C	2.56	0.46
1:A:44:VAL:CG1	1:A:45:GLY:N	2.79	0.46
1:A:184:GLU:CG	1:A:185:ASN:N	2.79	0.46
1:A:242:ASN:HD22	1:A:243:ASN:N	2.13	0.46
1:A:300:GLU:HG3	1:A:301:ASN:N	2.29	0.46
1:A:450:ASP:O	1:A:450:ASP:CG	2.58	0.46
1:A:646:THR:O	1:A:650:VAL:HG23	2.16	0.46
1:A:713:ILE:HD11	1:A:769:LEU:HD21	1.97	0.46
2:B:150:GLU:O	2:B:151:ASP:C	2.58	0.46
3:C:12:ARG:NH1	3:C:65:LEU:CD2	2.78	0.46
1:A:79:PRO:HG2	1:A:82:PHE:CD1	2.50	0.46
1:A:84:MET:N	1:A:84:MET:HE2	2.31	0.46
1:A:528:LYS:HA	1:A:529:PRO:HD3	1.81	0.46
1:A:551:LYS:HE2	1:A:555:TYR:CE1	2.51	0.46
1:A:572:LYS:O	1:A:573:ALA:HB3	2.16	0.46
2:B:29:ARG:O	2:B:31:GLY:N	2.49	0.46
2:B:132:LEU:O	2:B:133:LYS:HG2	2.15	0.46
1:A:15:LEU:HD12	1:A:15:LEU:HA	1.83	0.46
1:A:398:LEU:O	1:A:402:LEU:HB2	2.16	0.46
1:A:422:VAL:HG23	1:A:423:THR:N	2.31	0.46
1:A:190:ILE:HG23	1:A:254:ILE:CD1	2.46	0.46
1:A:712:ARG:HG2	1:A:763:PHE:CD2	2.51	0.46
1:A:718:PHE:CE1	1:A:722:TYR:CD1	3.04	0.46
2:B:146:LYS:HD2	2:B:146:LYS:HA	1.39	0.46
3:C:84:ALA:O	3:C:85:ASP:C	2.59	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:ALA:O	1:A:100:LEU:HB3	2.16	0.46
1:A:450:ASP:OD1	1:A:452:LYS:CG	2.63	0.46
2:B:130:ALA:HA	2:B:131:PRO:HD3	1.75	0.46
2:B:132:LEU:HD23	2:B:137:PHE:HA	1.97	0.46
1:A:1:MET:O	1:A:2:THR:OG1	2.26	0.46
1:A:572:LYS:O	1:A:572:LYS:CG	2.52	0.46
2:B:81:THR:O	2:B:82:ASP:C	2.58	0.46
1:A:615:SER:O	1:A:616:LYS:C	2.59	0.45
1:A:836:LYS:C	1:A:838:LEU:H	2.24	0.45
2:B:28:ASP:O	2:B:30:ASP:N	2.49	0.45
1:A:192:TYR:CE1	1:A:196:VAL:HG11	2.50	0.45
1:A:200:LEU:HD13	1:A:259:GLN:OE1	2.17	0.45
1:A:392:VAL:HG12	1:A:393:ASN:N	2.31	0.45
1:A:31:LYS:O	1:A:32:LYS:HG2	2.17	0.45
1:A:240:THR:H	1:A:284:GLU:HG2	1.81	0.45
1:A:258:THR:O	1:A:258:THR:CG2	2.63	0.45
1:A:280:GLN:CB	1:A:320:GLY:N	2.80	0.45
1:A:384:GLU:HA	1:A:387:ALA:HB3	1.98	0.45
1:A:425:SER:OG	1:A:605:ASN:ND2	2.50	0.45
1:A:690:LEU:O	1:A:693:LEU:N	2.50	0.45
1:A:779:ARG:HD2	1:A:779:ARG:HA	1.59	0.45
1:A:817:VAL:O	1:A:820:TRP:N	2.49	0.45
2:B:58:LEU:O	2:B:59:LYS:C	2.59	0.45
1:A:36:VAL:CG2	1:A:37:PRO:HD2	2.47	0.45
1:A:61:ASP:O	1:A:63:THR:N	2.48	0.45
1:A:88:MET:HE2	1:A:99:ILE:HA	1.93	0.45
1:A:163:MET:HE1	1:A:256:PHE:CD1	2.51	0.45
1:A:261:LYS:H	1:A:261:LYS:HG2	1.35	0.45
1:A:650:VAL:O	1:A:651:HIS:C	2.59	0.45
2:B:13:ARG:CD	2:B:13:ARG:H	2.29	0.45
1:A:142:GLY:HA2	1:A:161:GLN:HE21	1.79	0.45
1:A:289:ILE:O	1:A:289:ILE:HG12	2.16	0.45
1:A:608:VAL:HG12	1:A:612:LEU:CD1	2.47	0.45
1:A:767:GLY:O	1:A:768:VAL:C	2.59	0.45
1:A:805:ASP:O	1:A:808:ILE:HB	2.17	0.45
3:C:30:ALA:O	3:C:33:VAL:HG23	2.16	0.45
3:C:61:LYS:HG2	3:C:62:ALA:N	2.31	0.45
1:A:406:ILE:C	1:A:407:LYS:HD3	2.42	0.45
1:A:496:PHE:CD1	1:A:514:ASP:HA	2.51	0.45
1:A:659:MET:O	1:A:660:LYS:C	2.59	0.45
1:A:806:GLN:N	2:B:93:MET:HE1	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:136:ILE:CG2	3:C:137:ASP:N	2.76	0.45
3:C:143:GLU:O	3:C:144:ASP:C	2.60	0.45
1:A:346:THR:CG2	1:A:348:GLU:HB3	2.47	0.45
1:A:555:TYR:HD2	1:A:559:LEU:CD1	2.29	0.45
2:B:87:LEU:HB3	2:B:143:VAL:HG22	1.97	0.45
2:B:123:ILE:HG22	2:B:127:TRP:HE1	1.81	0.45
1:A:2:THR:HG21	1:A:143:LYS:CE	2.47	0.45
1:A:9:ASP:HB3	1:A:136:LEU:HD21	1.98	0.45
1:A:715:TYR:CZ	1:A:738:LYS:HG3	2.52	0.45
2:B:35:MET:O	2:B:38:LEU:HB2	2.17	0.45
2:B:144:ASP:O	2:B:145:ILE:C	2.58	0.45
1:A:176:GLY:O	1:A:182:LYS:HE3	2.17	0.45
1:A:363:LEU:HA	1:A:366:MET:SD	2.56	0.45
3:C:7:GLU:O	3:C:11:VAL:HG23	2.16	0.45
3:C:119:THR:CG2	3:C:120:GLU:N	2.79	0.45
1:A:35:TRP:HA	1:A:35:TRP:CE3	2.52	0.45
1:A:386:VAL:HG23	1:A:387:ALA:H	1.82	0.45
1:A:832:PHE:CZ	2:B:77:LYS:HD3	2.52	0.45
1:A:3:MET:HE1	1:A:14:CYS:HG	1.81	0.44
1:A:444:ARG:HD2	1:A:444:ARG:HA	1.48	0.44
1:A:524:GLU:O	1:A:528:LYS:HB2	2.18	0.44
1:A:546:SER:C	1:A:548:THR:N	2.71	0.44
1:A:388:PHE:O	1:A:389:LEU:C	2.60	0.44
1:A:619:ILE:O	1:A:619:ILE:CG2	2.65	0.44
1:A:709:PHE:CD2	1:A:765:LYS:HG2	2.52	0.44
1:A:794:TYR:CE1	3:C:152:GLY:C	2.94	0.44
1:A:836:LYS:HE3	2:B:17:GLU:CD	2.42	0.44
1:A:2:THR:CG2	1:A:143:LYS:HZ1	2.15	0.44
1:A:48:ILE:HA	1:A:58:VAL:HG22	2.00	0.44
1:A:407:LYS:O	1:A:408:VAL:CG2	2.63	0.44
1:A:440:TRP:CD1	1:A:621:LYS:CE	3.01	0.44
1:A:817:VAL:HA	2:B:146:LYS:CE	2.47	0.44
1:A:826:TRP:HB3	1:A:829:TRP:CB	2.47	0.44
1:A:836:LYS:HZ3	2:B:21:ALA:HB2	1.80	0.44
3:C:78:LYS:HE3	3:C:79:ASP:H	1.82	0.44
1:A:131:ILE:O	1:A:131:ILE:HG22	2.17	0.44
1:A:176:GLY:O	1:A:182:LYS:CE	2.65	0.44
1:A:529:PRO:O	1:A:530:MET:CB	2.66	0.44
1:A:604:ILE:H	1:A:644:PHE:HA	1.83	0.44
1:A:84:MET:HE2	1:A:84:MET:H	1.82	0.44
1:A:615:SER:O	1:A:620:VAL:HG22	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:48:VAL:O	2:B:50:PRO:HD3	2.17	0.44
3:C:44:PRO:CA	3:C:48:GLN:OE1	2.65	0.44
1:A:3:MET:HE1	1:A:10:MET:SD	2.58	0.44
1:A:199:SER:O	1:A:200:LEU:HD23	2.17	0.44
1:A:519:LEU:O	1:A:523:ILE:HG13	2.17	0.44
2:B:50:PRO:O	2:B:53:GLU:HB2	2.18	0.44
3:C:36:LEU:HD21	3:C:68:ILE:HD13	2.00	0.44
3:C:82:THR:HG21	3:C:87:PHE:CE2	2.53	0.44
3:C:117:ARG:H	3:C:117:ARG:HD2	1.83	0.44
1:A:6:SER:O	1:A:8:PRO:HD3	2.18	0.44
1:A:407:LYS:HB3	1:A:411:GLU:HG2	1.99	0.44
1:A:571:PRO:HD2	1:A:576:ALA:O	2.18	0.44
2:B:28:ASP:OD2	2:B:37:ASP:OD2	2.36	0.44
1:A:19:LYS:O	1:A:22:GLU:HB3	2.18	0.44
1:A:153:PHE:CD2	1:A:192:TYR:HD2	2.35	0.44
1:A:351:LEU:CD2	1:A:355:LYS:HE3	2.45	0.44
2:B:53:GLU:C	2:B:55:ASN:N	2.75	0.44
2:B:139:TYR:C	2:B:141:LYS:N	2.76	0.44
1:A:65:GLU:HA	1:A:65:GLU:OE1	2.18	0.43
1:A:101:HIS:O	1:A:102:ASN:C	2.60	0.43
1:A:280:GLN:HB2	1:A:319:GLN:CB	2.42	0.43
1:A:351:LEU:CG	1:A:355:LYS:HE3	2.48	0.43
1:A:786:MET:CE	3:C:82:THR:OG1	2.66	0.43
2:B:151:ASP:N	2:B:151:ASP:OD1	2.51	0.43
3:C:12:ARG:O	3:C:13:GLU:C	2.60	0.43
1:A:148:MET:HE3	1:A:148:MET:HB3	1.74	0.43
1:A:392:VAL:HG11	1:A:611:LEU:CG	2.48	0.43
1:A:495:MET:HE2	1:A:704:ILE:CG2	2.48	0.43
2:B:147:GLY:O	2:B:148:LYS:CG	2.66	0.43
1:A:450:ASP:C	1:A:452:LYS:N	2.75	0.43
1:A:794:TYR:OH	3:C:153:PRO:HA	2.18	0.43
3:C:46:GLU:O	3:C:47:ALA:C	2.57	0.43
1:A:285:ARG:CG	1:A:291:TYR:CE1	3.00	0.43
1:A:563:PRO:HG2	1:A:564:MET:H	1.82	0.43
1:A:78:ASN:HD21	1:A:91:LEU:HB3	1.82	0.43
1:A:247:ARG:HD2	1:A:247:ARG:HA	1.85	0.43
1:A:253:ARG:O	1:A:265:ALA:HA	2.18	0.43
1:A:290:PHE:CB	1:A:317:ILE:HD11	2.47	0.43
1:A:298:PHE:N	1:A:299:PRO:HD3	2.33	0.43
1:A:449:LEU:O	1:A:451:THR:N	2.50	0.43
1:A:482:TYR:OH	1:A:527:GLU:HG2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:722:TYR:O	1:A:723:SER:C	2.61	0.43
1:A:751:ASP:OD1	1:A:752:PRO:HD2	2.19	0.43
1:A:784:ILE:O	1:A:788:GLN:HG3	2.18	0.43
1:A:812:LEU:O	1:A:816:ASN:HB2	2.19	0.43
2:B:29:ARG:HH22	2:B:35:MET:H	1.62	0.43
1:A:49:GLN:OE1	1:A:49:GLN:HA	2.19	0.43
1:A:321:THR:CG2	1:A:322:LEU:H	2.32	0.43
1:A:382:GLU:H	1:A:382:GLU:HG3	1.39	0.43
1:A:559:LEU:HD23	1:A:559:LEU:HA	1.43	0.43
1:A:574:GLY:C	1:A:576:ALA:N	2.75	0.43
1:A:817:VAL:O	1:A:820:TRP:HB3	2.18	0.43
1:A:832:PHE:CE2	2:B:77:LYS:NZ	2.71	0.43
2:B:77:LYS:HE3	2:B:77:LYS:HB2	1.80	0.43
3:C:57:LYS:HG2	3:C:60:GLU:OE2	2.18	0.43
1:A:56:VAL:CG1	1:A:57:THR:N	2.81	0.43
1:A:106:ARG:O	1:A:111:PHE:HB2	2.19	0.43
1:A:380:THR:O	1:A:380:THR:HG22	2.18	0.43
1:A:424:ASN:O	1:A:425:SER:C	2.62	0.43
1:A:494:HIS:O	1:A:495:MET:C	2.62	0.43
1:A:32:LYS:HD3	1:A:48:ILE:O	2.18	0.43
1:A:51:THR:O	1:A:52:LYS:HB2	2.17	0.43
1:A:292:GLN:C	1:A:333:MET:HE3	2.43	0.43
1:A:293:LEU:HD13	1:A:305:ILE:HD11	2.00	0.43
1:A:542:PHE:O	1:A:543:PRO:C	2.62	0.43
1:A:709:PHE:HB3	1:A:763:PHE:HB3	2.00	0.43
1:A:711:ASN:HB2	1:A:764:PHE:HB2	2.00	0.43
3:C:93:THR:CG2	3:C:94:PHE:CD1	3.02	0.43
1:A:34:CYS:HB2	1:A:75:GLY:O	2.19	0.43
1:A:120:CYS:CB	1:A:155:ILE:CD1	2.96	0.43
1:A:569:LYS:O	1:A:570:PRO:C	2.61	0.43
1:A:771:MET:HE2	1:A:771:MET:HB3	1.67	0.43
2:B:101:PHE:HD2	2:B:139:TYR:CE2	2.36	0.43
3:C:78:LYS:HG3	3:C:79:ASP:H	1.83	0.43
3:C:89:GLU:HA	3:C:89:GLU:OE1	2.19	0.43
1:A:69:VAL:HG12	1:A:70:LYS:N	2.34	0.43
1:A:440:TRP:HZ2	1:A:444:ARG:NH1	2.17	0.43
1:A:721:ARG:NH2	1:A:773:GLU:OE2	2.47	0.43
1:A:816:ASN:ND2	2:B:82:ASP:HB2	2.32	0.43
1:A:3:MET:HE3	1:A:10:MET:SD	2.58	0.42
1:A:63:THR:O	1:A:64:GLN:O	2.37	0.42
1:A:250:LYS:HE3	1:A:252:ILE:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:ILE:HG22	1:A:307:ALA:O	2.19	0.42
1:A:615:SER:O	1:A:616:LYS:O	2.37	0.42
1:A:707:LYS:O	1:A:765:LYS:NZ	2.48	0.42
2:B:32:PHE:O	2:B:37:ASP:OD2	2.37	0.42
2:B:145:ILE:O	2:B:148:LYS:HG2	2.19	0.42
3:C:40:LEU:HD13	3:C:72:TYR:CE1	2.54	0.42
1:A:56:VAL:HG12	1:A:58:VAL:HG23	2.01	0.42
1:A:118:LEU:HD13	1:A:494:HIS:HD2	1.84	0.42
1:A:305:ILE:O	1:A:306:LEU:CG	2.66	0.42
1:A:381:ALA:O	1:A:384:GLU:HG2	2.19	0.42
1:A:418:ASN:OD1	1:A:418:ASN:C	2.61	0.42
1:A:800:TYR:CE1	3:C:17:LEU:CD2	3.02	0.42
2:B:101:PHE:CE1	2:B:138:ASN:OD1	2.72	0.42
1:A:96:GLU:O	1:A:97:ALA:C	2.62	0.42
1:A:437:MET:HA	1:A:622:MET:HE3	2.00	0.42
1:A:437:MET:HG3	1:A:622:MET:CE	2.50	0.42
1:A:584:HIS:O	1:A:585:TYR:C	2.60	0.42
1:A:661:ASN:O	1:A:665:THR:HG23	2.20	0.42
1:A:723:SER:C	1:A:725:LEU:N	2.75	0.42
3:C:82:THR:HG21	3:C:87:PHE:CZ	2.54	0.42
1:A:346:THR:HG22	1:A:348:GLU:N	2.30	0.42
1:A:659:MET:HE1	1:A:662:LEU:HD12	2.01	0.42
1:A:805:ASP:C	2:B:93:MET:HE1	2.44	0.42
1:A:826:TRP:O	1:A:828:TRP:N	2.52	0.42
1:A:407:LYS:C	1:A:408:VAL:HG23	2.45	0.42
1:A:557:ASN:HB3	1:A:558:HIS:CD2	2.54	0.42
2:B:24:MET:O	2:B:25:ILE:C	2.60	0.42
2:B:39:LYS:CE	2:B:54:LEU:HD22	2.50	0.42
2:B:56:ALA:HA	2:B:59:LYS:CG	2.48	0.42
3:C:99:GLN:OE1	3:C:99:GLN:HA	2.20	0.42
1:A:6:SER:O	1:A:7:ASP:C	2.63	0.42
1:A:258:THR:O	1:A:258:THR:HG22	2.18	0.42
1:A:348:GLU:O	1:A:351:LEU:HB3	2.20	0.42
1:A:488:GLN:O	1:A:491:PHE:HB3	2.19	0.42
1:A:567:LYS:HA	1:A:580:PHE:HA	2.02	0.42
1:A:660:LYS:HD2	1:A:660:LYS:O	2.19	0.42
1:A:736:ASP:OD1	1:A:738:LYS:N	2.52	0.42
1:A:800:TYR:CZ	1:A:804:GLN:NE2	2.84	0.42
1:A:816:ASN:ND2	2:B:87:LEU:HD21	2.34	0.42
2:B:91:PHE:O	2:B:92:SER:C	2.62	0.42
3:C:104:SER:HB3	3:C:140:ILE:HD11	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:TRP:CZ2	1:A:77:ARG:HG3	2.54	0.42
1:A:88:MET:HE1	1:A:99:ILE:HG23	2.02	0.42
1:A:220:LEU:O	1:A:221:GLU:C	2.61	0.42
1:A:362:HIS:O	1:A:365:GLU:N	2.43	0.42
2:B:25:ILE:HG21	2:B:33:ILE:HG23	2.02	0.42
2:B:32:PHE:O	2:B:33:ILE:C	2.61	0.42
3:C:119:THR:HG22	3:C:120:GLU:N	2.34	0.42
1:A:234:TYR:CE1	1:A:289:ILE:HD12	2.54	0.42
1:A:826:TRP:CZ2	2:B:60:GLU:OE1	2.73	0.42
3:C:102:ILE:HG13	3:C:142:TYR:CD2	2.52	0.42
1:A:118:LEU:CD1	1:A:494:HIS:HD2	2.33	0.42
1:A:236:ASN:HA	1:A:245:SER:O	2.20	0.42
1:A:367:LYS:O	1:A:368:TRP:CD2	2.73	0.42
1:A:187:LYS:O	1:A:191:GLN:HG3	2.19	0.42
1:A:267:ILE:N	1:A:446:ASN:OD1	2.43	0.42
1:A:440:TRP:CZ2	1:A:444:ARG:NH1	2.88	0.42
1:A:551:LYS:O	1:A:554:LEU:HB2	2.20	0.42
1:A:593:ILE:HD13	1:A:593:ILE:HA	1.80	0.42
1:A:612:LEU:HD23	1:A:612:LEU:HA	1.87	0.42
2:B:105:ASP:O	2:B:106:TYR:C	2.63	0.42
2:B:129:ASP:O	2:B:130:ALA:O	2.38	0.42
1:A:192:TYR:CE1	1:A:196:VAL:CG1	3.02	0.41
1:A:259:GLN:HB2	1:A:261:LYS:CD	2.40	0.41
1:A:298:PHE:O	1:A:299:PRO:C	2.63	0.41
1:A:363:LEU:O	1:A:426:ILE:HG21	2.20	0.41
2:B:131:PRO:HD2	2:B:137:PHE:HE1	1.79	0.41
3:C:29:ASP:O	3:C:32:LYS:N	2.53	0.41
1:A:280:GLN:HB3	1:A:320:GLY:HA3	2.02	0.41
1:A:828:TRP:NE1	2:B:60:GLU:OE1	2.53	0.41
2:B:74:PHE:CD2	2:B:77:LYS:NZ	2.84	0.41
2:B:106:TYR:O	2:B:110:LEU:HB2	2.19	0.41
3:C:20:PHE:CD2	3:C:20:PHE:C	2.99	0.41
1:A:58:VAL:O	1:A:66:THR:HA	2.20	0.41
1:A:374:GLN:CD	1:A:415:GLN:HG2	2.44	0.41
2:B:83:PRO:HD2	2:B:86:ALA:HB3	2.01	0.41
3:C:15:PHE:HE1	3:C:68:ILE:HD12	1.85	0.41
1:A:79:PRO:HG2	1:A:82:PHE:CE1	2.55	0.41
1:A:305:ILE:HG12	1:A:355:LYS:HA	2.03	0.41
1:A:484:ASN:O	1:A:485:GLU:C	2.63	0.41
1:A:542:PHE:O	1:A:545:ALA:N	2.36	0.41
1:A:693:LEU:HD22	1:A:698:VAL:HG11	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:792:ARG:NH2	3:C:117:ARG:O	2.53	0.41
3:C:120:GLU:HA	3:C:120:GLU:OE1	2.20	0.41
1:A:24:THR:O	1:A:24:THR:HG22	2.20	0.41
1:A:522:CYS:O	1:A:523:ILE:C	2.63	0.41
1:A:618:PRO:O	1:A:621:LYS:N	2.54	0.41
1:A:700:GLU:CD	1:A:703:ARG:HH11	2.28	0.41
1:A:746:SER:O	1:A:747:ALA:C	2.64	0.41
2:B:36:GLU:O	2:B:37:ASP:C	2.62	0.41
3:C:95:ASP:OD2	3:C:100:GLY:N	2.53	0.41
3:C:111:LEU:O	3:C:118:ILE:HB	2.19	0.41
3:C:117:ARG:CZ	3:C:117:ARG:HB3	2.50	0.41
1:A:2:THR:CG2	1:A:143:LYS:HZ3	2.30	0.41
1:A:464:ILE:HG23	1:A:465:ALA:H	1.80	0.41
1:A:820:TRP:CZ3	1:A:821:LEU:CD2	3.04	0.41
1:A:86:MET:HE2	1:A:150:PRO:HD3	2.02	0.41
1:A:369:LYS:HG3	1:A:370:GLN:N	2.36	0.41
1:A:665:THR:O	1:A:667:PRO:HD3	2.19	0.41
1:A:836:LYS:HG2	1:A:839:LEU:HD21	2.02	0.41
1:A:193:PHE:CZ	1:A:459:ILE:HG21	2.56	0.41
1:A:258:THR:N	1:A:261:LYS:HE2	2.36	0.41
1:A:479:CYS:HB3	1:A:651:HIS:NE2	2.35	0.41
1:A:602:ASP:N	1:A:603:PRO:CD	2.84	0.41
1:A:796:MET:HE3	3:C:35:ASP:OD1	2.20	0.41
2:B:46:GLY:C	2:B:47:ARG:HG2	2.45	0.41
2:B:141:LYS:O	2:B:144:ASP:HB2	2.21	0.41
3:C:14:VAL:HG12	3:C:36:LEU:HD12	2.03	0.41
3:C:30:ALA:O	3:C:31:ALA:C	2.63	0.41
1:A:192:TYR:HE1	1:A:196:VAL:HG11	1.86	0.41
1:A:290:PHE:HB3	1:A:317:ILE:HD13	2.00	0.41
1:A:305:ILE:O	1:A:306:LEU:HB2	2.19	0.41
1:A:372:GLY:O	1:A:373:GLU:HG3	2.20	0.41
1:A:393:ASN:O	1:A:395:GLY:N	2.54	0.41
1:A:412:TYR:CG	1:A:413:VAL:N	2.89	0.41
1:A:525:LEU:HD21	1:A:565:PHE:HB2	2.03	0.41
1:A:809:GLY:O	1:A:812:LEU:HB2	2.21	0.41
1:A:820:TRP:CB	2:B:146:LYS:HZ2	2.34	0.41
3:C:132:ILE:CD1	3:C:145:LEU:CD1	2.98	0.41
3:C:141:LYS:HD2	3:C:144:ASP:OD2	2.21	0.41
1:A:51:THR:O	1:A:52:LYS:CB	2.68	0.41
1:A:132:TYR:CZ	1:A:188:LYS:HD3	2.56	0.41
1:A:279:TYR:C	1:A:280:GLN:NE2	2.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:ALA:C	1:A:298:PHE:CG	2.98	0.41
1:A:569:LYS:HA	1:A:570:PRO:HD2	1.69	0.41
1:A:718:PHE:CE1	1:A:722:TYR:HD1	2.39	0.41
1:A:810:LEU:HD12	1:A:810:LEU:HA	1.92	0.41
2:B:131:PRO:HB3	2:B:141:LYS:CG	2.50	0.41
3:C:92:LYS:O	3:C:93:THR:C	2.64	0.41
1:A:40:ASP:CB	1:A:41:PHE:HD2	2.34	0.40
1:A:200:LEU:CD1	1:A:259:GLN:O	2.68	0.40
1:A:238:LYS:HD2	1:A:324:VAL:HG22	2.04	0.40
1:A:280:GLN:CB	1:A:319:GLN:HB2	2.45	0.40
1:A:645:GLN:HB3	1:A:646:THR:H	1.63	0.40
3:C:61:LYS:HB2	3:C:61:LYS:HE3	1.89	0.40
1:A:26:ILE:HB	1:A:27:PRO:CD	2.50	0.40
1:A:141:ARG:NH1	1:A:199:SER:OG	2.53	0.40
1:A:181:GLY:O	1:A:185:ASN:HB2	2.22	0.40
1:A:299:PRO:O	1:A:302:ILE:HB	2.21	0.40
1:A:380:THR:O	1:A:380:THR:CG2	2.70	0.40
1:A:412:TYR:CE2	1:A:413:VAL:O	2.74	0.40
1:A:528:LYS:HD2	1:A:529:PRO:HD2	2.03	0.40
3:C:12:ARG:NH1	3:C:65:LEU:HD23	2.36	0.40
1:A:369:LYS:CG	1:A:370:GLN:N	2.84	0.40
1:A:815:ARG:NH2	2:B:82:ASP:OD1	2.52	0.40
2:B:116:ASP:OD2	3:C:24:ARG:NH2	2.55	0.40
2:B:123:ILE:HG23	2:B:127:TRP:HE1	1.86	0.40
3:C:132:ILE:CD1	3:C:145:LEU:HD13	2.52	0.40
1:A:450:ASP:OD1	1:A:450:ASP:C	2.64	0.40
1:A:479:CYS:SG	1:A:651:HIS:CD2	3.14	0.40
1:A:572:LYS:O	1:A:574:GLY:N	2.48	0.40
1:A:787:PHE:O	1:A:788:GLN:C	2.64	0.40
2:B:35:MET:HE2	2:B:35:MET:HB3	1.64	0.40
1:A:112:ILE:HG21	1:A:125:PRO:HB3	2.03	0.40
1:A:236:ASN:HD22	1:A:244:ASN:HD21	1.67	0.40
1:A:358:GLY:HA2	1:A:361:LEU:HD12	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:16:GLN:OE1	2:B:68:THR:OG1[2_556]	2.10	0.10

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	802/839 (96%)	625 (78%)	109 (14%)	68 (8%)	0	4
2	B	143/153 (94%)	89 (62%)	26 (18%)	28 (20%)	0	0
3	C	154/159 (97%)	130 (84%)	17 (11%)	7 (4%)	2	13
All	All	1099/1151 (96%)	844 (77%)	152 (14%)	103 (9%)	0	3

All (103) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	8	PRO
1	A	52	LYS
1	A	61	ASP
1	A	62	LYS
1	A	65	GLU
1	A	131	ILE
1	A	178	SER
1	A	201	ALA
1	A	240	THR
1	A	275	SER
1	A	306	LEU
1	A	309	PRO
1	A	313	LEU
1	A	366	MET
1	A	380	THR
1	A	394	ALA
1	A	404	PRO
1	A	408	VAL
1	A	415	GLN
1	A	417	ARG
1	A	570	PRO
1	A	571	PRO
1	A	576	ALA

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Mol	Chain	Res	Type
1	A	616	LYS
2	B	9	LYS
2	B	27	GLN
2	B	48	VAL
2	B	99	GLN
2	B	117	ASN
2	B	130	ALA
2	B	134	ASN
2	B	148	LYS
2	B	150	GLU
3	C	2	GLN
3	C	24	ARG
3	C	136	ILE
3	C	139	ASN
1	A	5	PHE
1	A	15	LEU
1	A	127	ARG
1	A	145	ARG
1	A	274	LYS
1	A	296	PRO
1	A	312	GLY
1	A	317	ILE
1	A	346	THR
1	A	363	LEU
1	A	416	GLY
1	A	450	ASP
1	A	530	MET
1	A	644	PHE
1	A	679	LYS
1	A	827	GLU
2	B	25	ILE
2	B	30	ASP
2	B	54	LEU
2	B	59	LYS
2	B	66	ASN
2	B	84	GLU
2	B	98	GLY
2	B	125	ASN
3	C	82	THR
3	C	155	PRO
1	A	14	CYS
1	A	105	SER

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Mol	Chain	Res	Type
1	A	282	SER
1	A	350	LYS
1	A	406	ILE
1	A	514	ASP
1	A	532	ILE
1	A	681	PRO
1	A	823	LEU
2	B	42	PHE
2	B	51	ASP
2	B	79	SER
2	B	104	GLU
2	B	146	LYS
3	C	60	GLU
1	A	55	GLU
1	A	64	GLN
1	A	199	SER
1	A	403	LYS
1	A	465	ALA
1	A	475	PHE
1	A	543	PRO
1	A	556	ASP
1	A	732	SER
1	A	835	VAL
2	B	33	ILE
2	B	49	PRO
2	B	53	GLU
1	A	7	ASP
1	A	606	GLU
1	A	619	ILE
1	A	696	ASN
2	B	29	ARG
1	A	329	ASP
1	A	568	PRO
2	B	80	GLY
1	A	298	PHE
1	A	229	PRO
2	B	147	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar

resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	704/731 (96%)	642 (91%)	62 (9%)	9	32
2	B	128/134 (96%)	107 (84%)	21 (16%)	2	11
3	C	134/137 (98%)	121 (90%)	13 (10%)	8	28
All	All	966/1002 (96%)	870 (90%)	96 (10%)	7	27

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	CYS
1	A	36	VAL
1	A	39	PRO
1	A	41	PHE
1	A	68	VAL
1	A	144	ARG
1	A	182	LYS
1	A	188	LYS
1	A	217	LYS
1	A	246	SER
1	A	271	LEU
1	A	275	SER
1	A	282	SER
1	A	289	ILE
1	A	293	LEU
1	A	295	SER
1	A	296	PRO
1	A	302	ILE
1	A	313	LEU
1	A	317	ILE
1	A	340	PHE
1	A	382	GLU
1	A	403	LYS
1	A	407	LYS
1	A	410	THR
1	A	413	VAL
1	A	417	ARG
1	A	423	THR
1	A	425	SER
1	A	426	ILE

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Mol	Chain	Res	Type
1	A	448	THR
1	A	451	THR
1	A	480	ILE
1	A	508	ILE
1	A	511	GLU
1	A	529	PRO
1	A	532	ILE
1	A	535	ILE
1	A	543	PRO
1	A	546	SER
1	A	548	THR
1	A	549	SER
1	A	556	ASP
1	A	559	LEU
1	A	564	MET
1	A	583	HIS
1	A	593	ILE
1	A	620	VAL
1	A	621	LYS
1	A	622	MET
1	A	624	PHE
1	A	644	PHE
1	A	667	PRO
1	A	698	VAL
1	A	702	ILE
1	A	705	CYS
1	A	714	ILE
1	A	732	SER
1	A	765	LYS
1	A	815	ARG
1	A	822	VAL
1	A	827	GLU
2	B	9	LYS
2	B	15	MET
2	B	17	GLU
2	B	20	GLU
2	B	22	PHE
2	B	26	ASP
2	B	29	ARG
2	B	35	MET
2	B	38	LEU
2	B	45	LEU

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Mol	Chain	Res	Type
2	B	48	VAL
2	B	58	LEU
2	B	59	LYS
2	B	66	ASN
2	B	81	THR
2	B	107	LEU
2	B	113	ASN
2	B	124	LYS
2	B	134	ASN
2	B	142	MET
2	B	143	VAL
3	C	4	THR
3	C	8	ILE
3	C	44	PRO
3	C	68	ILE
3	C	77	SER
3	C	78	LYS
3	C	92	LYS
3	C	103	SER
3	C	107	ILE
3	C	109	ASN
3	C	117	ARG
3	C	118	ILE
3	C	149	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	ASN
1	A	158	ASN
1	A	161	GLN
1	A	242	ASN
1	A	244	ASN
1	A	288	HIS
1	A	301	ASN
1	A	362	HIS
1	A	415	GLN
1	A	439	ASN
1	A	447	GLN
1	A	484	ASN
1	A	494	HIS
1	A	558	HIS

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Mol	Chain	Res	Type
1	A	600	ASN
1	A	605	ASN
1	A	607	ASN
1	A	613	GLN
1	A	651	HIS
1	A	696	ASN
1	A	711	ASN
1	A	806	GLN
1	A	816	ASN
1	A	833	ASN
2	B	14	GLN
2	B	55	ASN
2	B	89	ASN
2	B	134	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	SO4	A	1001	-	4,4,4	0.30	0	6,6,6	0.09	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1001	SO4	4	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	808/839 (96%)	0.10	15 (1%) 66 48	13, 64, 137, 163	0
2	B	145/153 (94%)	0.43	3 (2%) 63 44	34, 100, 146, 163	0
3	C	156/159 (98%)	-0.08	4 (2%) 57 38	13, 47, 106, 152	0
All	All	1109/1151 (96%)	0.12	22 (1%) 65 46	13, 66, 140, 163	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	77	LYS	4.4
1	A	835	VAL	3.5
1	A	543	PRO	3.5
3	C	85	ASP	3.4
1	A	322	LEU	3.4
3	C	139	ASN	3.2
1	A	624	PHE	3.1
2	B	58	LEU	2.8
1	A	154	SER	2.8
1	A	622	MET	2.7
1	A	832	PHE	2.7
3	C	138	GLY	2.6
3	C	82	THR	2.5
1	A	366	MET	2.3
1	A	836	LYS	2.3
1	A	293	LEU	2.2
1	A	238	LYS	2.2
2	B	81	THR	2.1
1	A	612	LEU	2.1
1	A	541	MET	2.1
1	A	9	ASP	2.0
1	A	838	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	SO4	A	1001	5/5	0.89	0.12	58,58,58,58	5
5	CA	C	2001	1/1	0.95	0.10	58,58,58,58	0

6.5 Other polymers [i](#)

There are no such residues in this entry.